Processes Altering Charge State in Collisions of Hydrogen Atoms with H_2 Molecules

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The cross sections of all the elementary processes altering the charge states in the interaction $\vec{H}^0$—H_2 were determined by simultaneous mass analysis of the atomic particles formed in a single $\vec{H}^0$—H_2 collision and recording these particles by the coincidence technique.[1,2] The energy T_0 of the incident fast hydrogen atoms was varied within the range 5–50 keV. It was found that the principal contribution to the formation of slow H_2^+ and H^+ ions was made by the ionization processes, i.e., the processes in which one or two electrons were detached from the target molecule without altering the charge state of the fast particle ($\vec{H}^0$). The relative populations of the electron states of the target molecule ($1s\sigma_g$, $2p\sigma_u$, and excited electron states of the H_2^+ ion, as well as the state formed by two protons $H^+ + H^+$) were found to be practically equal for the ionization of the $\vec{H}^0$ atom and the electron capture by this atom. However, in the ionization of the molecule accompanied by simultaneous stripping of the incident $\vec{H}^0$ atom the population of the upper states ($2p\sigma_u$ and $H^+ + H^+$) was higher. The direct transfer of the kinetic energy from the incident particle to the nucleus of the target molecule made a significant contribution to the processes of dissociation of this molecule. This transfer effect was most pronounced in elementary processes of ionization and dissociation in the $\vec{H}^+$—H_2 case and of stripping accompanied by ionization and dissociation in the $\vec{H}^0$—H_2 case.

I. INTRODUCTION

COLLISIONS between a fast hydrogen atom and a hydrogen molecule ($\vec{H}^0 - H_2$)[1)] can give rise to various electron transitions in the target molecule and these transitions may alter the charge state of this molecule. The various possibilities include the formation of a molecular ion H_2^+, the dissociation of this ion into a hydrogen atom H^0 and a proton H^+ in various electron states, and finally, the formation of a pair of slow protons from the H_2 molecule. Such changes in the charge state of the target molecule may result from the ionization (the incident atom retains its charge state $\vec{H}^0$), the electron capture (the atom is transformed to a negative ion $\vec{H}^-$), and the stripping (the atom loses an electron and transforms into a proton $\vec{H}^+$). The present paper reports a study of elementary processes in which the charge state is altered, i.e., in the processes in which the charges and the masses of all the interacting atomic particles (atoms or atomic and molecular ions) are definite before and after a collision. A direct study of these processes requires simultaneous mass analysis of the fast (incident) and the slow (formed from the target molecule) particles. This has become possible because of the use of the coincidence method in investigations of atomic collisions.[1,2]

The cross sections of elementary processes resulting in changes of the charge state in the interaction $\vec{H}^0 - H_2$ were determined for incident-atom energies of 5–50 keV. Table I lists the various processes involved. An analysis of the kinetic energies of the protons resulting from the dissociation of the target molecule enabled us to identify and measure the cross sections of elementary processes differing not only in the sequence of changes in the charge states (processes 1–9 in Table I) but also of those processes which can be described by the same equation although they involve electron transitions into different states of the H_2^+ ion (processes 2a and 2b, 5a and 5b, 8a and 8b). We used a beam of hydrogen atoms in the 1s state. This beam was generated by charge exchange between protons with a given energy in a xenon gas target. After passing through this target the fast-particle beam was subjected to an electric field $\sim 4 \times 10^4$ V/cm in which the metastable atoms were reduced to the ground state and the highly excited atoms were ionized[3] and removed from the beam together with the residual protons. The cross sections of elementary processes were measured by employing a method similar to that which we used in an earlier study of the interaction of protons with hydrogen molecules.[4] All the data on the cross sections given in the present paper are calculated per one molecule.

Elementary processes resulting in changes in charge states in $\vec{H}^0 - H_2$ collisions

Process No.	Equation	Final state of target	Energy of slow ions (eV)	Cross section of process	Designation of process
1	$\vec{H}^0 + H_2 \to \vec{H}^0 + H_2^+ + e$	$1s\sigma_g$	~0	$\sigma^{00}_{0H_2^+}$	Ionization
2a	$\vec{H}^0 + H_2 \to \vec{H}^0 + H^+ + H^0 + e$	$1s\sigma_g$	~0	$\sigma^{00}_{0H^+H\mid 1s\sigma_g}$	Ionization and dissociation
2b		$2p\sigma_u$	~7	$\sigma^{00}_{0H^+H\mid 2p\sigma_u}$	
3	$\vec{H}^0 + H_2 \to \vec{H}^0 + H^+ + H^+ + 2e$	$H^+ + H^+$	~9	$\sigma^{00}_{02H^+}$	Double ionization
4	$\vec{H}^0 + H_2 \to \vec{H}^+ + H_2^+ + 2e$	$1s\sigma_g$	~0	$\sigma^{01}_{0H_2^+}$	Stripping and ionization
5a	$\vec{H}^0 + H_2 \to \vec{H}^+ + H^+ + H^0 + 2e$	$1s\sigma_g$	~0	$\sigma^{01}_{0H^+H\mid 1s\sigma_g}$	
5b		$2p\sigma_u$	~7	$\sigma^{01}_{0H^+H\mid 2p\sigma_u}$	
6	$\vec{H}^0 + H_2 \to \vec{H}^+ + H^+ + H^+ + 3e$	$H^+ + H^+$	~9	$\sigma^{01}_{02H^+}$	Stripping and double ionization
7	$\vec{H}^0 + H_2 \to \vec{H}^- + H_2^+$	$1s\sigma_g$	~0	$\sigma^{0-1}_{0H_2^+}$	Electron capture
8a	$\vec{H}^0 + H_2 \to \vec{H}^- + H^+ + H^0$	$1s\sigma_g$	~0	$\sigma^{0-1}_{0H^+H\mid 1s\sigma_g}$	Electron capture and dissociation
8b		$2p\sigma_u$	~7	$\sigma^{0-1}_{0H^+H\mid 2p\sigma_u}$	
9	$\vec{H}^0 + H_2 \to \vec{H}^- + H^+ + H^+ + e$	$H^+ + H^+$	~9	$\sigma^{0-1}_{02H^+}$	Electron capture and ionization

[1)]The arrow above a chemical symbol indicates a fast particle.

II. RESULTS OF MEASUREMENTS

1. Total Cross Sections of Formation of H_2^+ and H^+ Ions from H_2 Molecules

We determined first the total cross sections of formation of H_2^+ and H^+ ($\sigma_{0H_2^+}$ and σ_{0H^+}, respectively) in the interaction $\vec{H}^0 - H_2$. This was done by using the well-known method of analysis of the charge state of slow ions.[5] The results of this analysis are presented in Fig. 1. This figure includes also (for the sake of comparison) the data on the analogous cross sections for the $\vec{H}^+ - H_2$ interaction. The total cross sections of formation of the H_2^+ and H^+ ions in the $\vec{H}^0 - H_2$ case were found to increase with increasing energy T_0 of the incident hydrogen atoms right up to energies of $T_0 \sim 16-20$ keV at which these cross sections reached their maximum values (1.4×10^{-16} cm^2 for the formation of the H_2^+ ions and $\sim 2 \times 10^{-17}$ cm^2 for the H^+ ions). It is evident from Fig. 1 that in the $T_0 \approx 10-20$ keV range, where the curves of Fig. 1 have their maxima, the cross sections of formation of slow ions in the $\vec{H}^+ - H_2$ collisions are approximately one order of magnitude larger than the cross sections of formation of the same ions in the $\vec{H}^0 - H_2$ collisions. The cross sections decrease at higher values of the energy T_0 and the rate of decrease of the cross sections of formation of slow ions for the $\vec{H}^0 - H_2$ interaction is considerably slower than for the $\vec{H}^+ - H_2$ case. Consequently, when the incident-atom energy reaches $T_0 = 50$ keV the cross sections of formation of the slow H_2^+ and H^+ ions in the $\vec{H}^+ - H_2$ interaction are only three times as large as in the $\vec{H}^0 - H_2$ case.

A comparison of the cross sections obtained for $\vec{H}^0 - H_2$ case in[6] with the results obtained in the present investigation shows that although the cross sections of formation of the slow H_2^+ ions are in good agreement ($\sigma_{0H_2^+}$, curves 1 and 3), there is a considerable divergence between the cross sections of formation of the slow protons H^+ (σ_{0H^+}, curves 2 and 4), which amounts to a factor of 5 at $T_0 \approx 10$ keV. This can be explained by the incomplete extraction from the collision chamber of the protons with an initial kinetic energy of several electron-volts (Table I) in the experiments reported in[6].

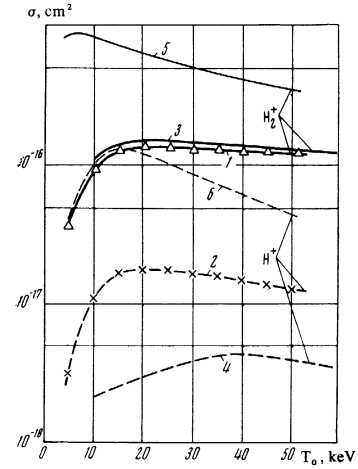

FIG. 1. Total cross sections of formation of slow H_2^+ (continuous curves) and H^+ (dashed curves) ions from H_2 molecules in $\vec{H}^0-H_2$ and $\vec{H}^+-H_2$ collisions. The slow ions are identified in the figure. The data for the $\vec{H}^0-H_2$ pair (thick curves) were obtained in the present investigation (1 and 2) or taken from [6] (3 and 4). The data for the $\vec{H}^+-H_2$ pair (thin curves were taken from [4] (5 and 6).

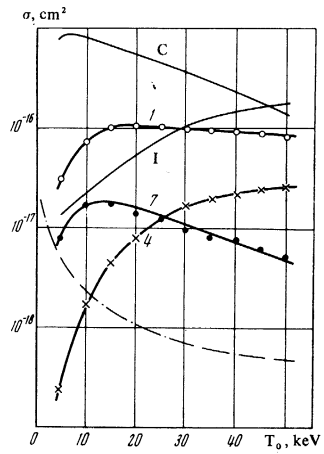

FIG. 2. Cross sections of elementary processes of formation of molecular H_2^+ ions from H_2 molecules. The following designations are used for the $\vec{H}^0-H_2$ pair: 1) ionization, $\sigma^{00}_{0H_2^+}$; 7) electron capture, $\sigma^{0-1}_{0H_2^+}$; 4) stripping and ionization, $\sigma^{01}_{0H_2^+}$ (the numbers alongside the curves represent the processes listed in Table I). The designations used for the $\vec{H}^+-H_2$ pair (the data are taken from [4]) are: I) ionization, $\sigma^{11}_{0H_2^+}$; c) capture (charge exchange, $\sigma^{10}_{0H_2^+}$. The chain curve represents the calculated cross section σ_{Coul} for the transfer of energy necessary for the dissociation of H_2^+ ions from the $1s\sigma_g$ state in the case of Coulomb interaction between the incident hydrogen particle and the nuclei of the H_2 molecule.

2. Cross Sections of Elementary Processes Involving Changes in Charge States

A. Processes leading to the formation of H_2^+ molecular ions. The values of the cross sections $\sigma^{0m}_{0H_2^+}$ (m is the charge of the fast particle after a collision, which can be +1, 0, and −1) are given in Fig. 2. Three processes lead to the formation of the H_2^+ molecular ions: the ionization ($\sigma^{00}_{0H_2^+}$, process 1 in Table I), the stripping accompanied by ionization ($\sigma^{01}_{0H_2^+}$, process 4), and the electron capture ($\sigma^{0-1}_{0H_2^+}$, process 7), The same figure includes, for the sake of comparison, the cross sections of the processes leading to the formation of the H_2^+ ions as a result of the $H^+ - H_2$ collisions: the electron capture $\sigma^{10}_{0H_2^+}$ ($\vec{H}^+ + H_2 \rightarrow \vec{H}^0 + H_2^+$) and the ionization $\sigma^{11}_{0H_2^+}$ ($\vec{H}^+ + H_2 \rightarrow \vec{H}^+ + H_2^+ + e$).[4] As mentioned earlier, the total cross section of formation of H_2^+ ions in the H_2^+ ions in the $\vec{H}^+ - H_2$ collisions is considerably larger than in the $\vec{H}^0 - H_2$ case [$\sigma_{0H_2^+}(\vec{H}_+)$ $> \sigma_{0H_2^+}(\vec{H}^0)$]. It is evident from Fig. 2, which gives the cross sections of the elementary processes contributing to the total cross section $\sigma_{0H_2^+}$ that at the incident-particle energies in the range $T_0 < 25$ keV this difference between the total cross sections is due to the large electron-capture (charge-exchange) cross section of the incident protons $\sigma^{10}_{0H_2^+}$ (curve C in Fig. 2), whereas at higher energies this difference is also related to the value of the ionization cross section $\sigma^{11}_{0H^+}$ (curve I in Fig. 2), which is greater than the ionization cross section $\sigma^{00}_{0H_2^+}$ in the $\vec{H}^0 - H_2$ case (curve 1).

The main contribution to the formation of the H_2^+ ions in the $\vec{H}^0 - H_2$ collisions is made by the ionization process (curve 1 in Fig. 2 and process 1 in Table I). The ionization cross section $\sigma^{00}_{0H_2^+}$ increases rapidly with increasing energy of the incident particles right up to $T_0 \sim 15$ keV. The largest value of this cross section (1.1×10^{-16} cm^2) is observed at $T_0 \sim 20$ keV. The ionization process in this range of

energies of the incident $\vec{H}^0$ hydrogen atoms produces over 75% of all the H_2^+ slow ions. The contribution of the stripping accompanied by ionization, represented by the cross section $\sigma^{01}_{0H_2^+}$ (curve 4 in Fig. 2 and process 4 in Table I), increases in importance at higher incident particle energies. The largest value of the cross section $\sigma^{01}_{0H_2^+}$ in the investigated range of energies is 2.7×10^{-17} cm^2 at $T_0 \approx 50$ keV. At low energies a considerable contribution to the formation of the H_2^+ ions is made by a different process which is the electron capture represented by the cross section $\sigma^{0-1}_{0H_2^+}$ (curve 7 in Fig. 2 and process 7 in Table I). The largest cross section of the electron-capture process (1.9×10^{-17} cm^2) is observed at $T_0 \approx 13$ keV.

B. Processes leading to the formation of protons from H_2 molecules. The data on the cross sections of all the elementary processes leading to the formation of slow protons as a result of the ionization (2a, 2b, and 3 in Table I), the stripping accompanied by ionization (5a, 5b, 6), and the electron capture (8a, 8b, 9) are plotted in Fig. 3. The ionization as well as the stripping or the electron capture accompanied by dissociation may be associated with three different types of electron transition from the ground state ($^1\Sigma_g^+$) of the H_2 target molecule:

1) to lower states ($1s\sigma_g$) of the H_2^+ ion, followed by dissociation of this ion into a proton and a hydrogen atom (curves 2a, 5a, and 8a in Fig. 3);

2) to repulsive states ($2p\sigma_u$) and to excited electron states of the H_2^+ ion (curves 2b, 5b, 8b), again followed by dissociation into a proton and an atom;

3) to the repulsive state $H^+ + H^+$ (curves 3, 6, 9), followed by dissociation into two protons.

If the electron transitions to the $1s\sigma_g$ state occur in accordance with the Franck-Condon principle, the main result is the formation of the H_2^+ molecular ions in various vibrational states. The dissociation of the H_2^+ ions from the $1s\sigma_g$ state occurs only when an electron transition takes place at the shortest possible internuclear distance r and the ground vibrational state of the target molecule H_2 is within a region of radius r. Under these conditions the energy of the molecular system is higher than the energy of the upper vibrational state ($1s\sigma_g$) of the H_2^+ ion and this leads to the dissociation into a proton and a hydrogen atom in the 1s state. The kinetic energy of the dissociation products in this process does not exceed several tens of electron-volts. The relative probability of such dissociation is low and it amounts to ~1% of the total probability of the electron transition to the $1s\sigma_g$ state. It is evident from Fig. 3 that the cross sections of formation of protons as a result of ionization, stripping and ionization, or electron capture followed by the dissociation of the H_2^+ ion from the $1s\sigma_g$ state (curves 2a, 5a, 8a in Fig. 3 and the corresponding processes in Table I) depend on the kinetic energy T_0 in a manner similar to the cross sections of the analogous processes which lead to the formation of the H_2^+ molecular ion (curves 1, 4, and 7 in Fig. 2 and processes 1, 4, and 7 in Table I). In contrast to the transitions to the $1s\sigma_g$ state, any transition to the $2p\sigma_u$ state and to all excited electron states of the H_2^+ ion unavoidably lead to dissociation ($H_2^+ \rightarrow H^0 + H^+$). The H^+ ions and the H^0 atoms formed in this way have wide and overlapping (for different electron states) distributions in the kinetic energy.[7]

The changes in the charge states of the particles on transition to the $2p\sigma_u$ state are the same as those observed for transitions to the excited electron states of the H_2^+ ion, with the exception of the electron state of the H^0 atom. Therefore, the cross sections of the elementary processes obtained in the present study for the dissociation $H_2^+ \rightarrow H^0 + H^+$, denoted arbitrarily by the symbol $2p\sigma_u$, represent electron transitions not only to the state $2p\sigma_u$ but also to all the excited electron states of the H_2^+ ion. It is evident from Fig. 3 that, as in the case of the slow H_2^+ ions, the greatest contribution to the formation of the H^+ ions is made by the ionization processes (2b, 3). The contribution of the stripping with ionization and the dissociation processes accompanied by the loss an electron by the fast atom ($\vec{H}^0 \rightarrow \vec{H}^+$, processes 5b and 6) is important only at high energies whereas the contribution of the processes involving the capture of one electron by the fast atom ($\vec{H}^0 \rightarrow \vec{H}^-$) followed by dissociation of the resultant H_2^+ molecular ion (8b) is important only at low energies.

An analysis of the processes of proton formation (Fig. 3) at high energies ($T_0 \gtrsim 40$ keV) shows that the cross sections of the processes involving the detachment of both electrons from the target molecule are larger than the cross sections of the processes involving the detachment of one electron although less energy is required for the latter process (this is evident from a comparison of the cross sections of the processes 2b and 3, 5b and 6, 8b and 9).

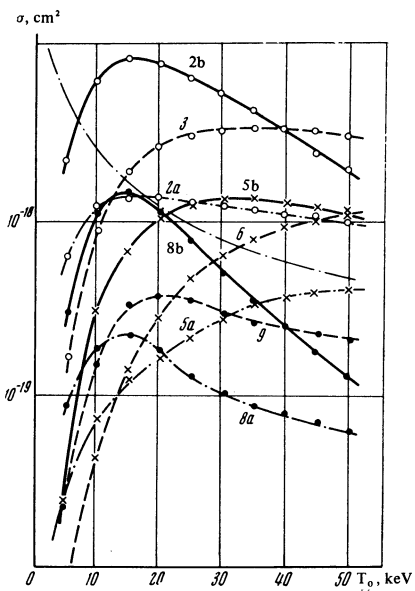

FIG. 3. Cross sections of elementary processes of formation of protons from H_2 molecules (the numbers alongside the curves represent the processes listed in Table I). ○) Ionization (2a, 2b, 3); X) stripping and ionization (5a, 5b, 6); ●) electron capture (8a, 8b, 9). The various processes associated with electron transitions are indicated as follows: the continuous curves (2b, 5b, 8b) represent transitions to the $2p\sigma_u$ and excited electron states of the H_2^+ ion; the dashed curves (3, 6, 9) to the $H^+ + H^+$ state; the thick chain curves (2a, 5a, 8a) to the $Is\sigma_g$ state; the thin chain curves represent σ_{Coul} (see caption of Fig. 2).

3. Relationship between Electron Transitions in the Target Molecule and Processes Leading to Changes in Charge States

Measurements of the cross sections of elementary processes make it possible to determine the interrelationships between the processes of ionization, electron capture, and stripping accompanied by ionization in the case of any specific electron transition in the target molecule. These measurements can be used also to determine the role of the various electron transitions in the target molecule in the realization of various elementary collision processes. Clearly, the relative probability of ionization, stripping with ionization, and electron capture for any specific electron transitions is determined directly by the charge states P_m of the fast particles after a collision, i.e., in the case when the incident particle is the hydrogen atom $\vec{H}^0$ this probability is governed by the relationship between the numbers of the fast $\vec{H}^0$ atoms (m = 0), of the fast $\vec{H}^+$ protons (m = +1), and of the fast negative $\vec{H}^-$ ions (m = −1). The curves plotted in Fig. 4 show the charge states of the fast particles after collisions in which electron transitions took place from the ground state ($^1\Sigma_g^+$) of the H_2 molecule to one of the following states: $1s\sigma_g$ without dissociation of the H_2^+ ion; $1s\sigma_g$ with such dissociation; $2p\sigma_u$ and excited electron states of H_2^+; and the state formed by two protons ($H^+ + H^+$). In spite of the large difference between the energies required for these electron transitions in the molecular system (~18 eV for the transition to the $1s\sigma_g$ state, ~28 eV for the transition to the $2p\sigma_u$ state, and ~45 eV for the formation of two protons $H^+ + H^+$), the charge states of the fast particles after a collision are basically the same in all cases. A similar dependence of the charge states of fast hydrogen particles on the energy lost in inelastic processes in the target particle was found in our earlier study of the collisions of $\vec{H}^+$, $\vec{H}^0$, and $\vec{H}^-$ particles with He atoms.[8]

It would be interesting to analyse the populations of the electron states of the molecular system after an elementary process of specified type. The relative probabilities of the electron transitions to the $1s\sigma_g$, $2p\sigma_u$, and $H^+ + H^+$ states in the target molecule are plotted in Fig. 5 for each of the following processes: ionization (1, 2a + 2b, 3 in Table I), stripping and ionization (4, 5a + 5b, 6), and electron capture (7, 8a ± 8b, 9). The most interesting is the observation that the relative probabilities of the electron transitions are practically equal for the ionization and capture processes. In fact, the populations of the states resulting from the capture and ionization in the energy range $T_0 > 15$ keV are identical for all the electron states: $1s\sigma_g$ (curves 7 and 1 in Fig. 5), $2p\sigma_u$ (curves 8b + 8a and 2b + 2a), and $H^+ + H^+$ (curves 9 and 3). On the other hand, the population of the $2p\sigma_u$ (curve 5a + 5b) and the $H^+ + H^+$ (curve 6) states after stripping accompanied by ionization is higher than after electron capture or the ionization.

4. Influence of Direct Transfer of Kinetic Energy to Nuclei of a Target Molecule in Dissociation Processes

The dissociation of a target molecule may result not only in the case of electron transitions to the repulsive states but also in the case of direct transfer of the kinetic energy to the nuclei of the molecule from the incident particle. This effect can be discovered by comparing the experimentally obtained dissociation probabilities with those calculated for transitions obeying the Franck-Condon principle. The influence of the transfer of the kinetic energy to the nuclei of the target molecule was observed in the investigations of Fogel' et al.,[9] who determined the populations of the rotational and the vibrational levels in the dissociation of N_2^+ ions formed as a result of atomic collisions. A similar effect was evidently found in a study of the formation of protons from H_2 molecules subjected to

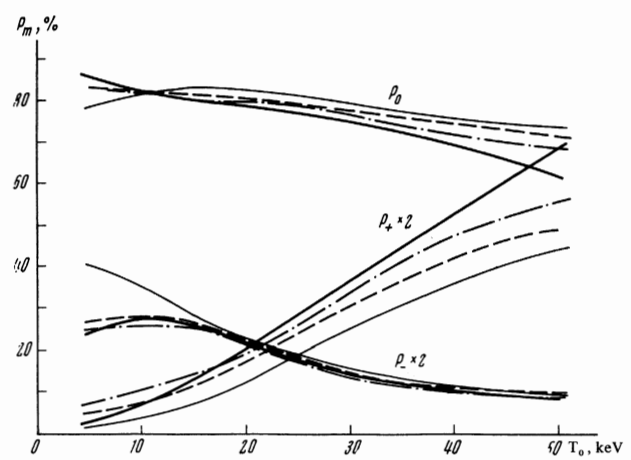

FIG. 4. Charge states P_0, P_+, and P_- of the fast particles after the $\vec{H}^0$-H_2 collision in the case of electron transitions to specific states of the target molecule: the thin continuous curves represent transitions to the $1s\sigma_g$ state without dissociation of the H_2^+ ion; the chain curves represent transitions to the $1s\sigma_g$ state accompanied by the dissociation $H_2^+ \rightarrow H^+ + H^0$; the thick continuous curves represent transitions to the $2p\sigma_u$ state; the dashed curves represent transitions to the $H^+ + H^+$ state.

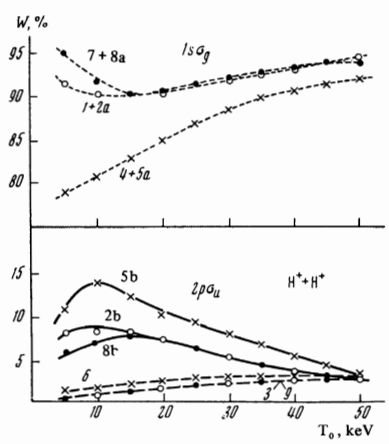

FIG. 5. Relative probabilities W of transitions to various electron states of the H_2^+ ion and to the $H^+ + H^+$ state plotted for the principal elementary processes: ○) ionization; ×) stripping and ionization; ●) electron capture. The numbers alongside the curves represent the processes listed in Table I. The dotted curves represent transitions to the $1s\sigma_g$ state the continuous curves to the $2p\sigma_u$ state, and the dashed curves to the $H^+ + H^+$ state.

bombardment with heavy particles.[10] When protons are produced from the H_2 molecule, we can find a process which is sensitive to the direct transfer of the kinetic energy: this is the transition $^1\Sigma_g^+ \rightarrow 1s\sigma_g$. When the Franck-Condon principle is obeyed, this transition leads mainly to the formation of the H_2^+ ions and only ~1% of the transitions result in the dissociation $H_2^+ \rightarrow H^0 + H^+$. In our investigation of the $\vec{H}^+ - H_2$ collisions[4] we determined the fraction of the H_2^+ ions dissociating in this way. This fraction was found to be independent of the incident-proton energy (5–50 keV) and close to the calculated values[11] and those obtained in electron bombardment,[12] in which the Franck-Condon principle was known to be obeyed.

A quantitative estimate of the influence of the deviation from the Franck-Condon principle on the dissociation processes occurring in the collisions of $\vec{H}^0$ and $\vec{H}^+$ with H_2 can be obtained by calculating the cross section for the transfer of the energy needed for the dissociation of the H_2^+ ion. Gerasimenko and Oksyuk[13] demonstrated that the quantum-mechanical and classical calculations of the probability of dissociation of a molecule give practically identical results provided the energy of the incident atomic particle is higher than 200 eV. If the dissociation energy D (in the system linked to the center of mass of the target molecule) is transferred by an incident hydrogen particle to one of the nuclei of the H_2 molecule at such distances that the screening by electrons can be ignored, the Coulomb collision cross section is given by

$$\sigma_{Coul} = \pi e^4 / T_0 D. \qquad (1)$$

In the range of the incident-particle energies (T_0 = 5–50 keV) used in the present investigation the maximum value of σ_{Coul} is $\sim 7 \times 10^{-18}$ cm^2 (Figs. 2 and 3). This means that in collisions leading to dissociation as a result of direct energy transfer the shortest distance between the particles does not exceed $r \sim 0.1$ Å. Calculations of the potential energy of H_2^+ ion[14] show that when the distance between protons ($r \sim 0.1$ Å) is much less than the internuclear separation in the H_2^+ ion, the forces due to the interaction between electrons and the protons are an order of magnitude weaker than the Coulomb repulsion between the protons. Under these circumstances we are justified in applying Eq. (1) to collisions of $\vec{H}^0$ and $\vec{H}^+$ with H_2 in the $T_0 \geq 5$ keV range.

It is evident from Fig. 2 that the cross section σ_{Coul} for the $\vec{H}^0 - H_2$ pair is comparable with the total cross section of formation of the H_2^+ ion, which consists of the cross sections of the processes 1, 4, 7 ($\sigma^{00}_{0H_2^+}$, $\sigma^{01}_{0H_2^+}$, $\sigma^{0-1}_{0H_2^+}$) and that σ_{Coul} is much smaller than the analogous cross section for the $H^+ - H_2$ pair which consists of the cross sections of the processes C and I ($\sigma^{10}_{0H_2^+}$, $\sigma^{11}_{0H_2^+}$). Consequently, the influence of the direct transfer of the kinetic energy on the dissociation probability can be observed only for the $\vec{H}^0 - H_2$ pair. Figure 6a shows the relative probability of the dissociation of the H_2^+ ion from the $1s\sigma_g$ state in the $\vec{H}^0 - H_2$ collisions obtained in the present investigation. This figure includes the corresponding dependence for the $\vec{H}^+ - H_2$ case, obtained by us in an earlier study[4] and refined in the present investigation. In contrast to the $\vec{H}^+ - H_2$ case, the probability of dissociation of the $H_2^+(1s\sigma_g)$ ion in the $\vec{H}^0 - H_2$ collisions increases when the energy T_0 is reduced. This increase is due to the direct transfer of the kinetic energy to the atoms in the target molecule.

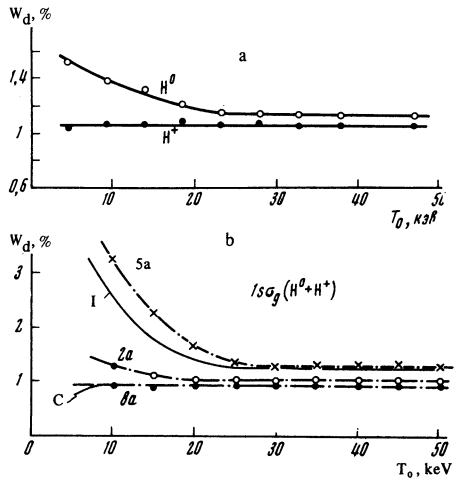

FIG. 6. a) Relative probabilities of dissociation W_d of H_2^+ ions formed as a result of $H_2(^1\Sigma_g^+) \rightarrow H_2^+(1s\sigma_g)$ electron transitions: ○) $\vec{H}^0$–H_2 pair; ●) $\vec{H}^+$–H_2 pair. [4] b) Relative probabilities of dissociation W_d of H_2^+ ions in the $1s\sigma_g$ state formed as a result of electron capture (8a), ionization (2a), and stripping-cum-ionization (5a) in the $\vec{H}^0$–H_2 collisions (Table I), and as a result of ionization (I) and electron capture (C) in the $\vec{H}^+$–H_2 collisions.

The results presented in Fig. 6a apply to the total probabilities of dissociation of the H_2^+ ions from the $1s\sigma_g$ state for the $\vec{H}^0 - H_2$ and $\vec{H}^0 - H_2$ pairs. It should be mentioned that the direct transfer of the kinetic energy may have different effects not only for different pairs of the colliding particles but also for different elementary processes in the same pair if these processes occur at different approach distances. Figure 6b shows the data obtained on the probability of dissociation of the $H_2^+(1s\sigma_g)$ ions formed as a result of elementary processes of capture, ionization, or stripping with ionization. It is evident from Fig. 6b that in the electron capture by protons (curve C) the fraction of the dissociating $H_2^+(1s\sigma_g)$ ions is independent of the incident proton energy T_0. The capture cross section in the $\vec{H}^+ - H_2$ case is quite large ($\sim 10^{-15}$ cm^2 for $T_0 \sim 5$ keV) and, consequently, the approach distances in collisions are also large. Therefore, the formation of protons as a result of dissociation of $H_2^+(1s\sigma_g)$ is solely due to electron transitions in which the Franck-Condon principle is obeyed. Similar results are obtained for the capture processes (8a) in the $\vec{H}^0 - H_2$ case although in this case the ion formation cross section is comparable with the cross section σ_{Coul}. However, in the ionization processes occurring in the $\vec{H}^0 - H_2$ (curve 2a) or $\vec{H}^+ - H_2$ (curve I) collisions, and particularly in the case of stripping-cum-ionization processes in the $\vec{H}^0 - H_2$ collisions (curve 5a), the fraction of the dissociating $H_2^+(1s\sigma_g)$ ions increases considerably when the energy T_0 is reduced.

In these cases the processes in question occur at closer approach distances between the particles and the dissociation results not only from electron transi-

tions but also from direct transfer of the kinetic energy to the atoms in the target molecule.

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