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Low energy fragments from O^{2+} + H_2 collisions following single and double electron removal from the target

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Synopsis Fragmentation of H_2 by 20-keV O^{2+} was studied. A time of flight setup was developed to measure the low-energy fragment ions originating from singly ionized target molecules. High-energy fragments stemming from double electron removal were measured by an electrostatic spectrometer. The contribution of the low-energy fragments is significant but smaller than that of the energetic ones. Though single electron removal is more probable it less likely leads to dissociation. A statistical type model shows a good agreement with the experimental results.

Ion-impact-induced fragmentation of molecules in the gas phase is a key process in astrophysical environments and may provide important information for radiolysis studies. Emission of low-energy fragment ions is a strong output channel following the excitation and moderate ionization of the target molecules. However, its experimental investigation is difficult since low energy ions are sensitive to disturbing electric fields.

A time-of-flight measuring device was developed at Atomki for studying fragment ions in the 0.1-2 eV energy range to extend the results for 20-keV O^{2+} + H_2 collisions obtained by an electrostatic spectrometer at Ganil [1]. The emitted ions fly through a well-shielded field-free region before their detection on a 2D position sensitive detector. Their energy can be determined from their flight times. The detector can be rotated around the center of the chamber, so the angular distribution of the ions can be determined as well in a wide range.

We measured the energy and angular distribution of the emitted protons. No significant anisotropy was observed except for increased background-like contribution around 90° observation angle due to binary knock out by the projectile.

The measured cross sections show a maximum in the 0.1-0.3 eV range, which is most likely due to dissociation of H_2^+ ions created by single electron capture from the target. This is in accordance with the results of a recent thermodynamic model for molecular collisions [2]. Single capture does not always lead to dissociation of H_2^+. Its ground state is stable, dissociation occurs if it was created with internuclear separation far from equilibrium. Our ab initio quasi-molecular calculations for single capture show an order of magnitude higher cross sections than for the observed total low-energy proton production indicating that dissociation is indeed only partial.

At higher energies, a peak appears at 9.7 eV due to Coulomb explosion of the doubly ionized hydrogen molecules. It corresponds to about 90 % of the emitted protons. The thermodynamic model reproduces the observed cross section. It shows that transfer ionization has a similar contribution to double electron removal from the target as double capture. The energy of the peak indicates that Coulomb explosion is initiated at nearly equilibrium internuclear separation of H_2. In experiments by O^{5+} projectiles, it was found that the internuclear separation changes during the collision process and it increases with decreasing impact energy [3]. The thermodynamic model shows peakshift of -0.9 eV compared to the experiment, indicating an overestimation of this effect. But its existence suggests that fragmentation efficiency in single electron removal, which is dependent on the internuclear separation, may be sensitive on projectile energy.

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