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Hydrogen migration observed in fragmentation of the pyridine molecules in collisions with the H^+ , H_2^+ , He^+ and He^{++} cations

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Synopsis The hydrogen atom migration preceding fragmentation of the pyridine molecules by the H^+ , H_2^+ , He^+ and He^{++} collisions has been investigated in the 5-2000 eV energy range. The pyridine molecule structure is lacking of the NH group, thus formation of the NH radicals is an evidence of the H atom relocation prior to the cation-induced fragmentation. The $NH(A^3\Pi)$ fragmentation yields measured by detecting its $A^3\Pi \rightarrow X^3\Sigma^-$ fluorescence show that it depends on the selected projectile and the projectile velocity.

Many investigations have been devoted to understanding of the molecular reaction dynamics and chemical reactivity of molecular systems. In particular, selectively induced and controlled chemical reactions in molecular collisions have been studied by several different techniques, including molecular dynamics of photoexcited molecules [1,2], mode-selective excitation in ultrafast laser pulses [3], and more recently by site- and bond-selective dissociation in potassium collisions with pyrimidine bases of DNA [4].

The H atom migration observed in fragmentation of the pyridine (C_5H_5N) molecules induced by the H^+ , H_2^+ , He^+ and He^{++} collisions has been studied experimentally using collision-induced luminescence spectroscopy [5]. The collision energies of the cations were varied between 5 and 2000 eV and thus covered a velocity range from 30 to 440 km/s depending on the projectile mass.

In Figure 1 the emission spectra obtained for the He^+ and He^{++} cations are presented. The NH radicals have been identified by recording the $A^3\Pi \rightarrow X^3\Sigma^-$ emission. The ring of the pyridine molecule is built from five CH units and one N heteroatom [6]. Therefore to generate NH, it should undergo molecular rearrangements associated with migration of the hydrogen atom to form the NH group. Based on *ab initio* molecular calculations the plausible mechanisms for the NH formation will be proposed.

Figure 2 displays the velocity dependences of the $NH(A^3\Pi)$ fragmentation yields obtained in the H^+ , H_2^+ and He^+ collisions. It is clearly seen that these functions have different shapes and in the case of H_2^+ and He^+ the $NH(A^3\Pi)$ production yields strongly depend on the cation velocity.

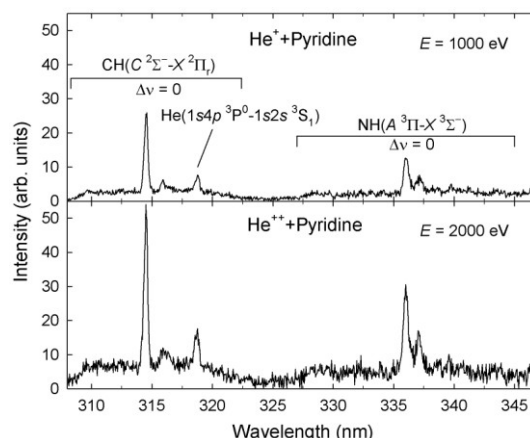


Figure 1. Emission spectra measured for He^+ and He^{++} collisions with the pyridine molecules.

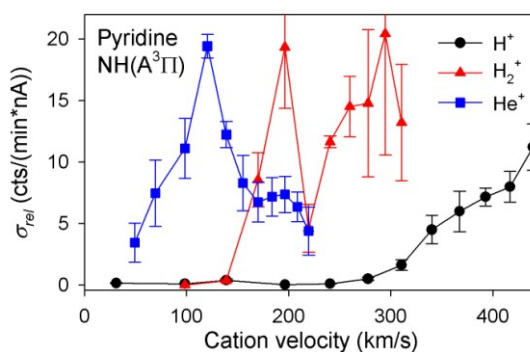


Figure 2. Fragmentation yields, σ_{rel} , of the excited $NH(A^3\Pi)$ fragments.

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