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Rapid formation of H_3^+ from ammonia and methane following ionization by fast protons¹

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Bond rearrangement, specifically the formation of H_2^+ and H_3^+ after ionization of methane and ammonia by 4 MeV protons, is studied in both the common and deuterated isotopes of those molecules. Our coincidence-time-of-flight measurements show the relative probability of H_2^+ and H_3^+ production from ammonia was higher for the lighter isotope, contradicting the common intuition that the rearrangement occurs on the timescale of the dissociation. The isotopic effects in methane, while smaller, were in the opposite direction. As expected, the relative probability of bond rearrangement leading to H_2^+ increases with the number of hydrogen atoms in the target for H_2O , NH_3 , and CH_4 targets. Formation of H_3^+ , however, is less likely from a methane target than from ammonia. We examined this result by calculating the ionic potential energy surface in reduced coordinates corresponding to a symmetric stretch of a H_3^+ triangle away from the nitrogen or carbon atom. From both the experiment and the model calculation, we find that bond rearrangement is a two step processes. First, the nuclear wavepacket is projected onto the ionic potential energy surface by a sudden (vertical) ionization, and then it propagates to the final products. The details of both steps determine the amount of bond rearrangement.

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