Isotopic effects in bond rearrangement caused by sudden ionization of ammonia and methane molecules

ELI PARKE, Kansas State University

The production of $\text{H}_2^+$ and $\text{H}_3^+$ fragments upon dissociation of ammonia and methane molecules involves rearrangements of the molecular bonds. Fast ion impact results in ionizations on time scales of 10 attoseconds, thus freezing the nuclear motion. Our earlier studies of $\text{H}_2^+$ formation upon dissociation of water molecules by fast ions showed a strong isotopic dependence. Recently, we measured isotopic effects in the production rate of $\text{H}_2^+$ and $\text{H}_3^+$ from $\text{NH}_3$ and $\text{CH}_4$ ionized by the same ions. Compared to $\text{H}_2^+$, creating $\text{H}_3^+$ requires the rapid cleavage and formation of additional bonds. The process is enhanced, however, by the geometrical similarity of the parent molecules and the triangle-shaped $\text{H}_3^+$ ions. Differences in triangle size result in vibrational excitation and may cause isotopic differences.

1Supported by the Chemical Sciences, Geosciences and Biosciences Division, Office of Basic Energy Sciences, Office of Science, U.S. Department of Energy, and by Research Corporation