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Electronic collisions with molecular cations: species relevant in the edge of the fusion plasma and plasma facing material in the fusion devices.

The impetus behind this abstract comes in relation to studies in experimental nuclear reactors with walls made up of materials containing simple atoms (e.g., Be, C, N), referred to as PFPs or plasma-facing materials, that may react with the fuel atoms (H, D, T) producing BeH, CH, NH, and their cations, all this related to the long-time elusive quest for controlled nuclear fusion energy employing magnetic-field confinement, particularly related to ITER. Generally, for kinetic modeling of low-temperature plasmas, it is not only essential to know all the constituent species present in the plasma but also the reaction rate coefficients (which can be obtained from cross sections) for dominant collision processes that are pathways to final products.

Molecular ions are a constituent of many low-temperature plasmas, where the collision of these ions with electrons plays an important role in governing their chemistry. Hydrocarbon ions, and in particular CH^+, are found in the edge plasmas in those fusion reactors operating with graphite or carbon fiber composite as plasma-facing material \cite{Tawara95}. Sometimes, these ions occur as an impurity in the plasma of fusion reactors operating with graphite as plasma-facing material and play a crucial role in understanding carbon erosion and redeposition. Collision cross sections for these processes are therefore important for modeling the plasma environment and understanding the chemistry of formation and destruction of CH^+ as well as the carbon erosion and redeposition in the plasma-facing components.

Many nitrogen plasmas contain NH^+, and therefore, the kinetic modeling of these plasmas requires cross-sections for different electron-induced processes in NH^+. NH^+ is also to be observed in a fusion plasma (or indeed any other sort of plasma, for example, ammonia plasmas), and it will be via emissions from its electronically excited states.

The competitive model of quantum mechanics can be used to describe Feshbach resonances, which are extremely excited bound states superposed with the continuum. Because they generate dissociation at low energy, these bound states are essential for explaining the dissociative recombination of the molecule that often occurs in this plasma environment. One effective theory that yields quantitative findings for identifying the interaction indicated by potential energy curves is the R-Matrix technique. The contribution of Feshbach resonances to the dissociation of molecules, as indicated by the dissociative rates, will be discussed in this presentation. The illustrations are based
on CH^+ \cite{Chakrabarti17}and NH^+ \cite{Ghosh22} cations and correspond to CH and NH molecules.

We have obtained a detailed construction of the potential energy curves for the ions CH^+, NH^+ and resonant states and corresponding their widths as the inter-nuclear distance R varies. Other collisional calculations should benefit from these resonant states, particularly the dissociative recombination of the CH^+ and NH^+ ions. Several resonant states of different symmetries, which were unknown till now, have been systematically identified and their widths calculated, which proved much more challenging due to the presence of many avoided crossings. It is hoped that the bound and the new resonant states obtained by us will open up other molecular dynamics studies so that the fusion devices can be improved in the future.

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