Energy deposit by electron excitation in CₙN⁺ projectiles (n=1-3) colliding at intermediate velocity with He atoms: semi-empirical estimates and calculations

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Synopsis
Using measured dissociation branching ratios and theoretical dissociation energies, we extracted semi-empirical estimates of the energy deposit due to electron excitation in CₙN⁺-He collisions at v=2.2 a.u. We compared these estimates to calculations based on the IAE (Independent Atom and Electron) model where the atom(ion)-atom excitation is treated within the Classical Trajectory Monte Carlo (CTMC) approach. A good agreement has been found. This atomic approach is also able to reproduce the experimental Kinetic Energy Release (KER) in CN⁺ dissociation measured in 3.5 a.u CN⁺-He collision.

Experiments have been performed at the Tandem accelerator in Orsay (France). We used the AGAT setup for excitation of the molecule and detection of its fragmentation. The way the internal energy distribution (IED) of the CₙN⁺ was derived from the fragmentation pattern has been explicated elsewhere [1]. KER measurements were performed using a dedicated position sensitive detector [2].

In the case of CN⁺ dissociation at v=3.5 a.u we measured the KER for both C⁺/N and C/N⁺ channels [2]. By assuming dissociation towards fragments in their electronic ground states to occur, we could reconstruct, using calculated dissociation energies, the internal energy of the molecule CN⁺ following electronic excitation. Results will be presented and compared to the IAE/CTMC calculation at the conference.

References

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Figure 1. Calculated internal energy deposit in C₂N⁺ following electron excitation

On the other hand, a IAE/CTMC calculation of the energy deposit resulting from atomic excitation was performed. The C₂N⁺ molecule was supposed to be made of independent atomic constituents colliding independently with He atoms. Excitation of atoms in final (n,l) levels were calculated with CTMC. Energies of final atomic excited states were obtained from NIST database. Figure 1 shows the internal energy deposit in C₂N⁺ calculated with the IAE/CTMC model. As will be shown at the conference, this distribution is compatible with the one obtained from fragmentation branching ratios [1].