Resonant electron-molecular cation collisions in the edge plasmas of fusion devices: new state-to-state cross sections and rate coefficients

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INTRODUCTION

The Multichannel Quantum Defect Theory (MQDT) [1] has been employed in computing cross sections and Maxwell rate coefficients for electron-driven reactions involving molecular cations. These data are appropriate for the modeling of the kinetics of various cold ionized media of fundamental interest, including the plasma-wall interaction [2].

Data on the following processes - among others – are needed [3]:

Dissociative Recombination (DR):

$$AB^{+}+e^{-}\rightarrow AB^{*},\ AB^{**}\rightarrow A+B,$$

Vibrational/Rotational Excitation (VE/RE), de-Excitation (VdE/RdE):

$$AB^{+}(N^{+},v^{+})+e^{-}\rightarrow AB^{*},\ AB^{**}\rightarrow AB^{+}(N^{+\prime},v^{+\prime})+e^{-}$$

Dissociative Excitation (DE):

$$AB^{+}+e^{-}\rightarrow AB^{**}\rightarrow A+B^{+}+e^{-}$$

RESULTS

Extensive cross sections and rate coefficients have been produced for the benchmark cation **HD^+** [4-6]. The role of the DE for the hydrogen isotopomers, and that of the core-excited Rydberg states, have been clearly put in evidence by an appropriate account of the mixing of the various reaction channels, open and closed. The calculated ro-vibrationally resolved state-to-state cross sections and/or rate coefficients have been averaged and compared with storage ring experimental results – **Figure 1**.

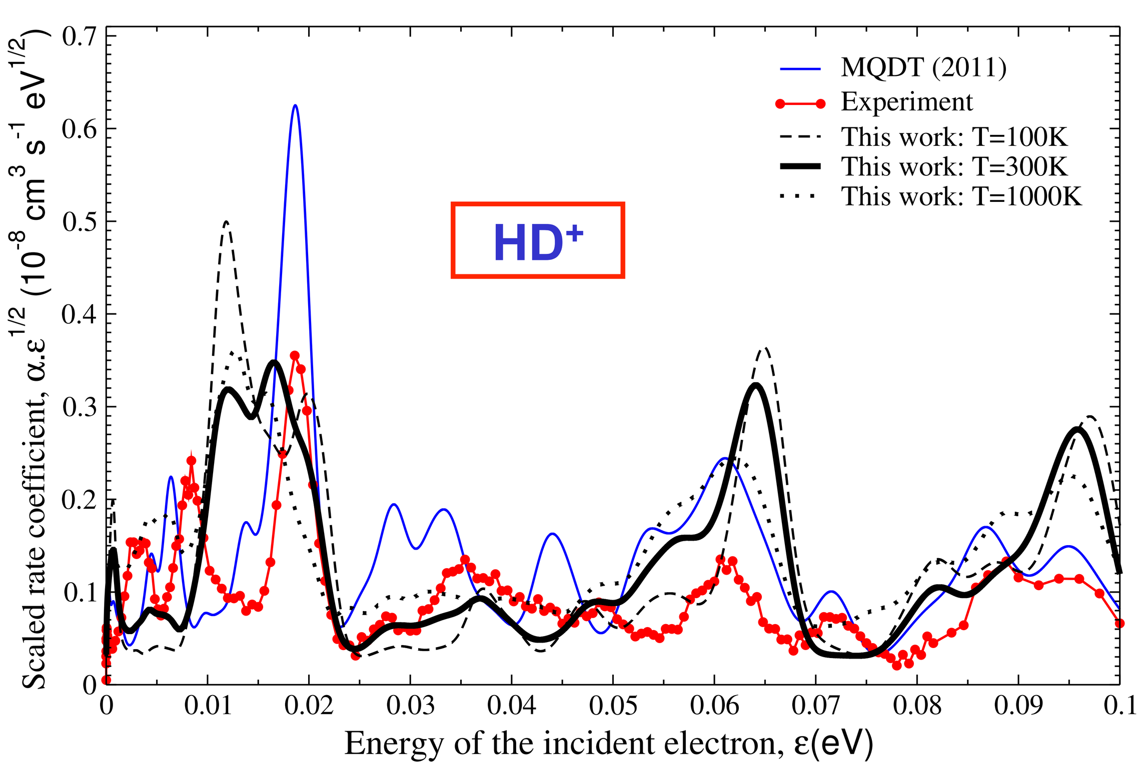

Figure 1. Rotationally-averaged Maxwell anisotropic rate coefficients for the dissociative recombination of HD^+, compared with TSR storage-ring measurements [4].

In order to provide collisional data for the modeling of the fusion edge plasmas and the primordial gas of the early Universe [7], extensive cross sections and rate coefficients have been produced for H_2^+ [8,9], some more recent results being illustrated in **Figure 2**.

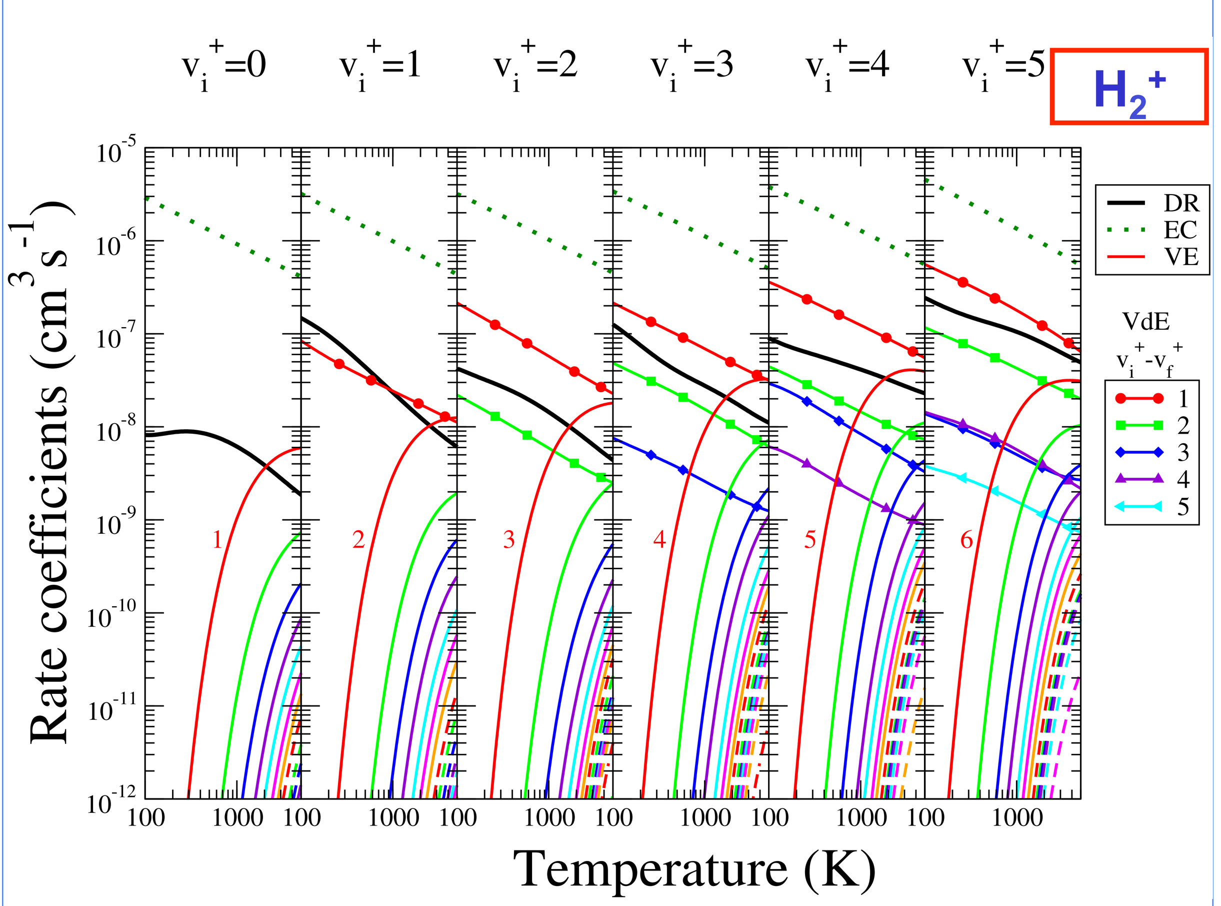

Figure 2. Maxwell isotropic rate coefficients for the DR, state-to-state VE, VdE and elastic collisions (EC) of electrons with the H_2^+ ion.

For the chemical modeling of edge fusion plasmas, extensive cross sections and rate coefficients have been produced for **BeH^+** ([10] – **Figure 3** and **4**). The role of the DE has been clearly put in evidence by an appropriate account of the mixing of the various reaction channels, open and closed [10]. The calculations have been performed for all the vibrational levels (v_i^+=0,…,17) of the target molecular ion.

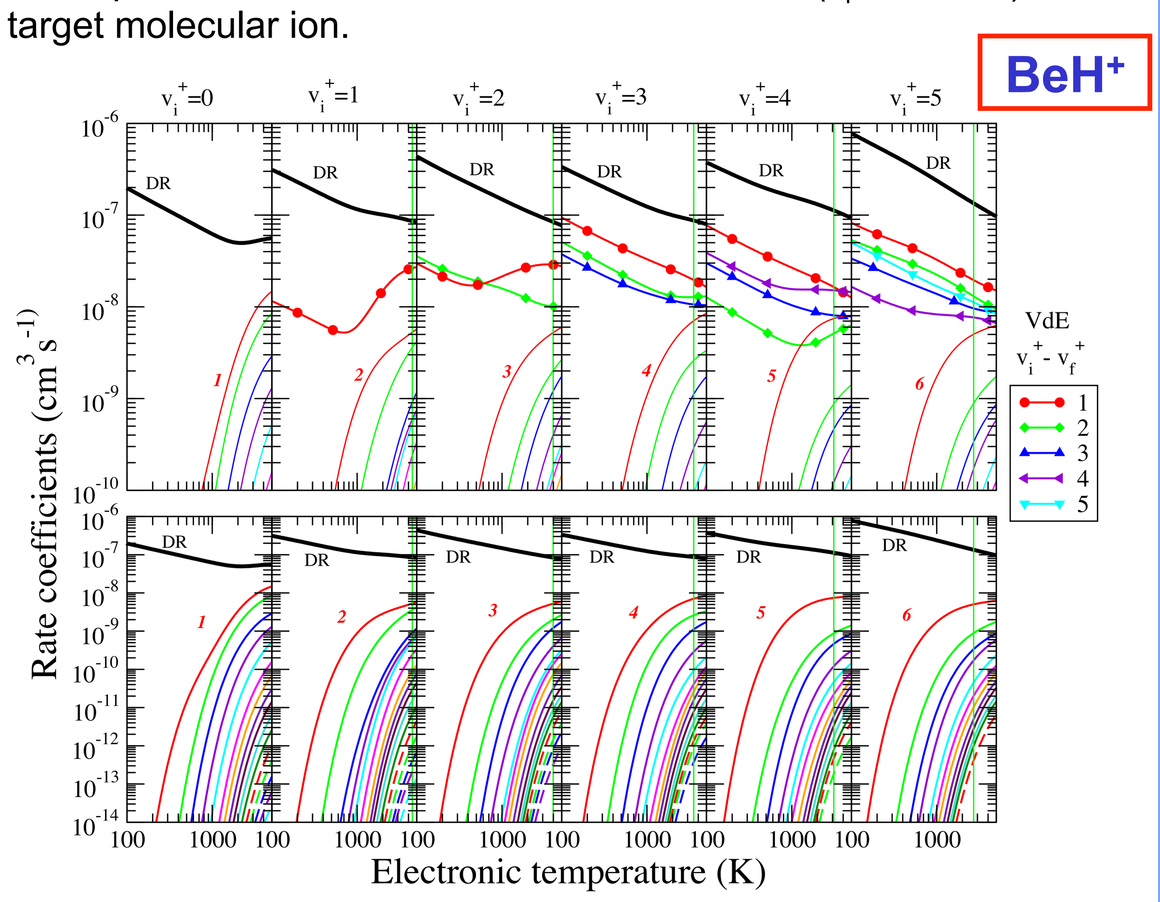

Figure 3. Maxwell rate coefficients for the DR, VE and VdE of BeH^+ ion in its electronic ground state and on its initial vibrational states v_i^+ [10]. The numbers label the final vibrational state of the transition.

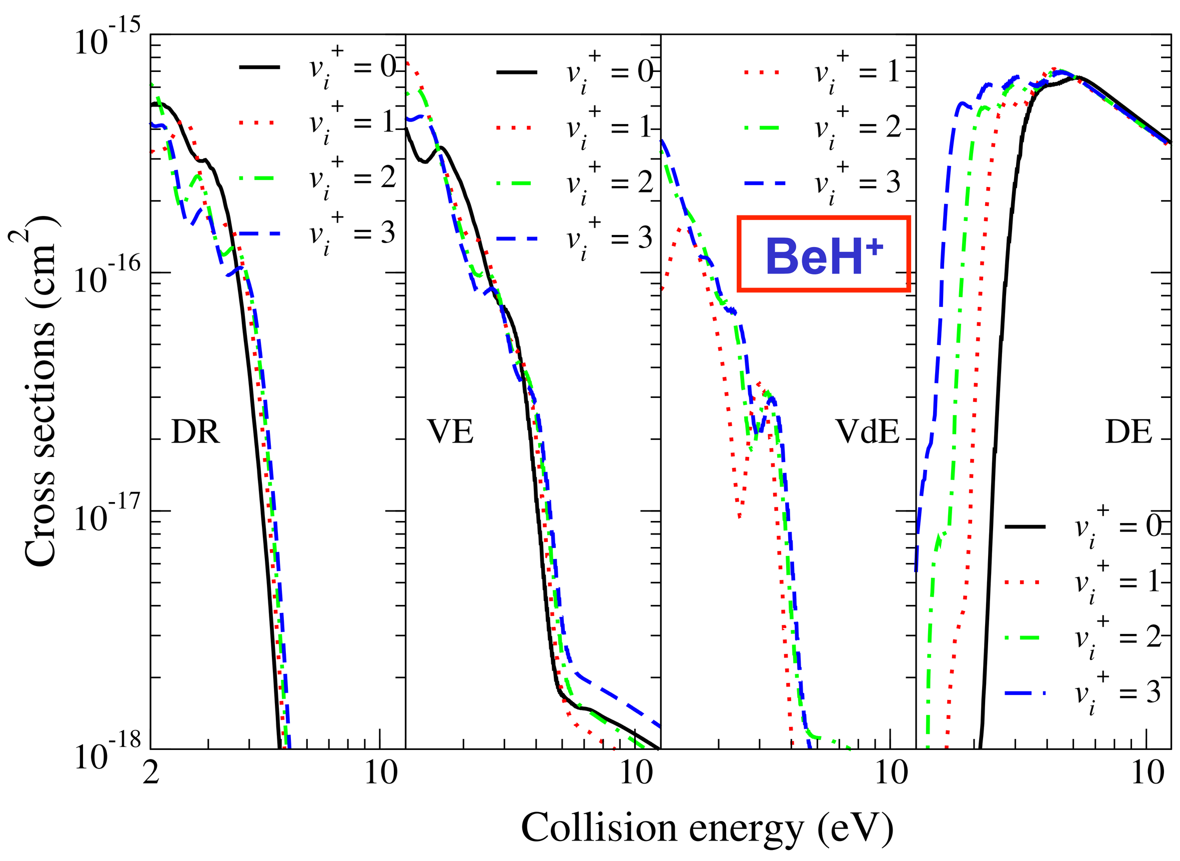

Figure 4. DR, VE, VdE and DE cross sections of the BeH^+ ion in its electronic ground state and on its initial vibrational states v_i^+ for collision energies ranging from 2 to 10 eV.

In order to complete the collisional data for the modeling of edge plasmas for fusion devices we have started on a comprehensive study on the **BeD^+** and **BeT^+** isotopomers. The first preliminary results on the DR, VE and VdE global rate coefficients illustrated in **Figure 5**, show the isotopic effect.

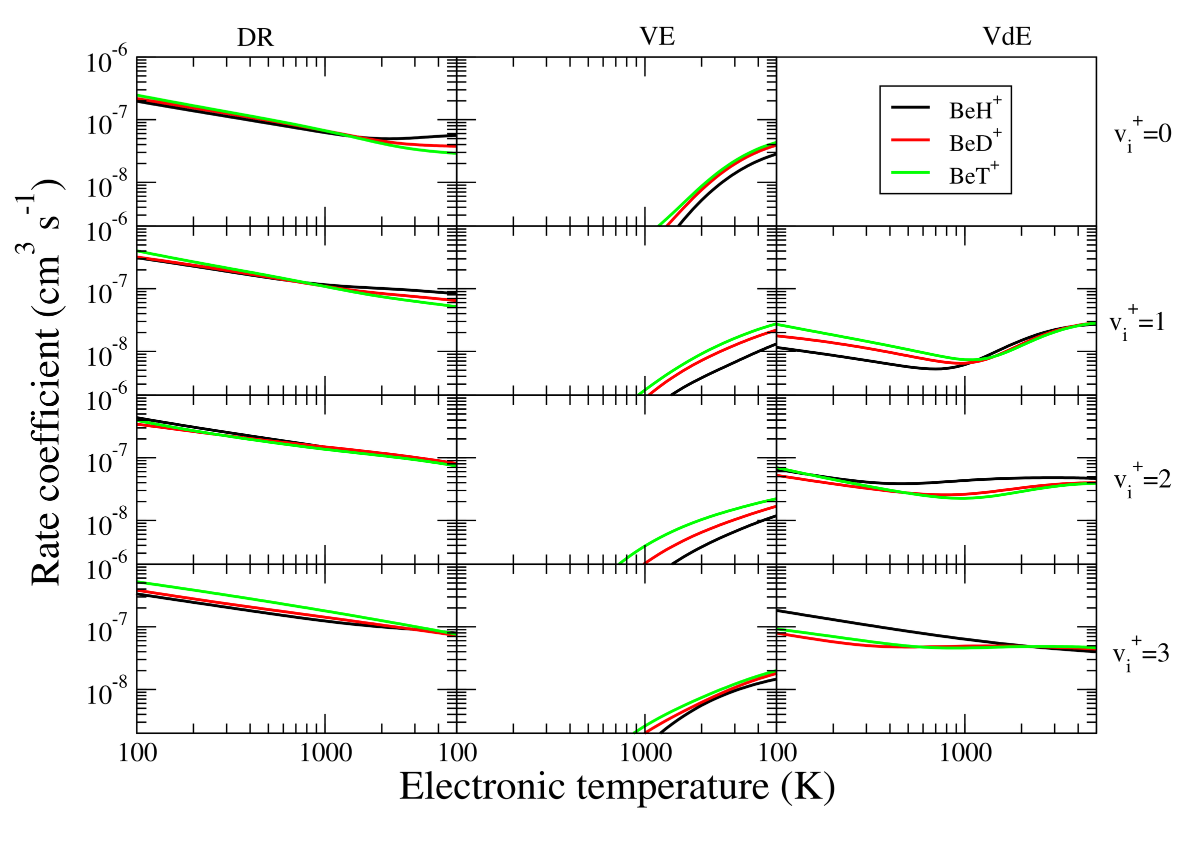

Figure 5. Global Maxwell rate coefficients for the DR, VE and VdE of BeH^+ ion and its isotopomers in their electronic ground states and on its lowest initial vibrational states v_i^+.

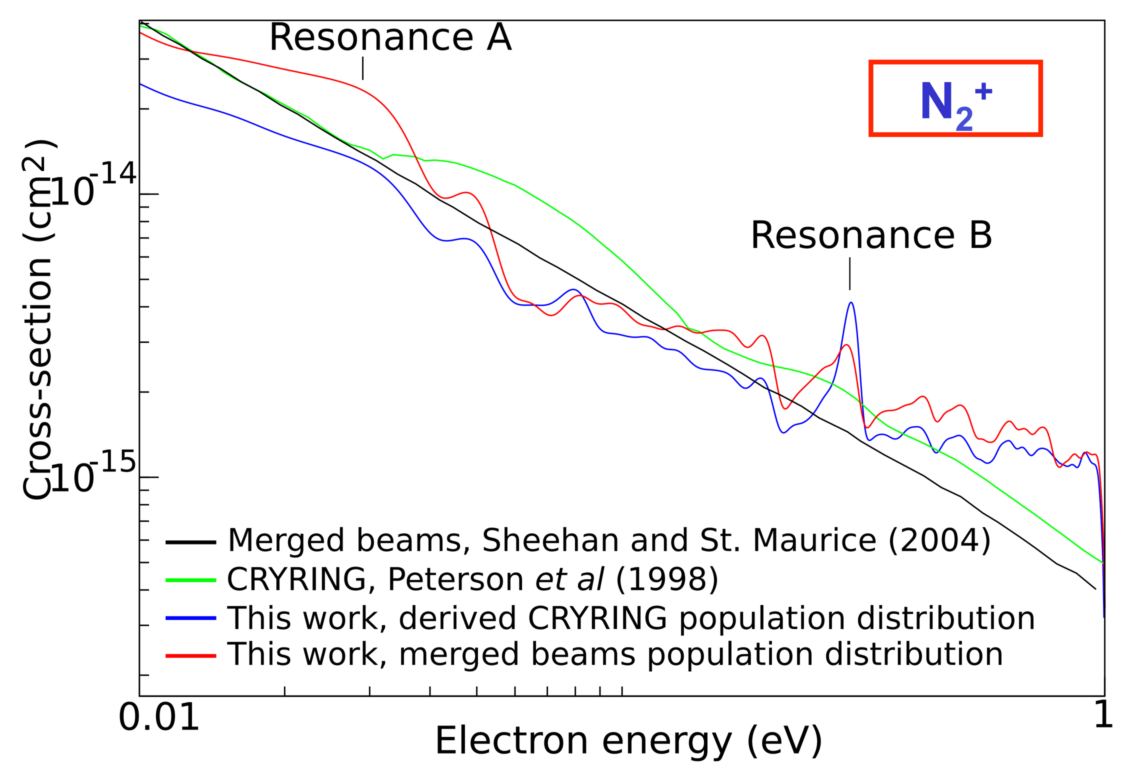

Figure 6. N_2^+ DR effective cross sections compared with those measured using CRYRING [12] and single-pass merged beams devices [13].

The core-excited effects have been included successfully in the study of the DR of N_2^+ [11] – **Figure 6** – occurring in the plasma torch aiming to assist the detritiation process of the Tokamak. Rate coefficients and branching ratios have been produced in satisfactory agreement with experiments [12,13].

The study performed on **CH^+** – **Figure 7** – reveals the importance of the excited cores and higher order theoretical treatment in order to achieve a realistic model.

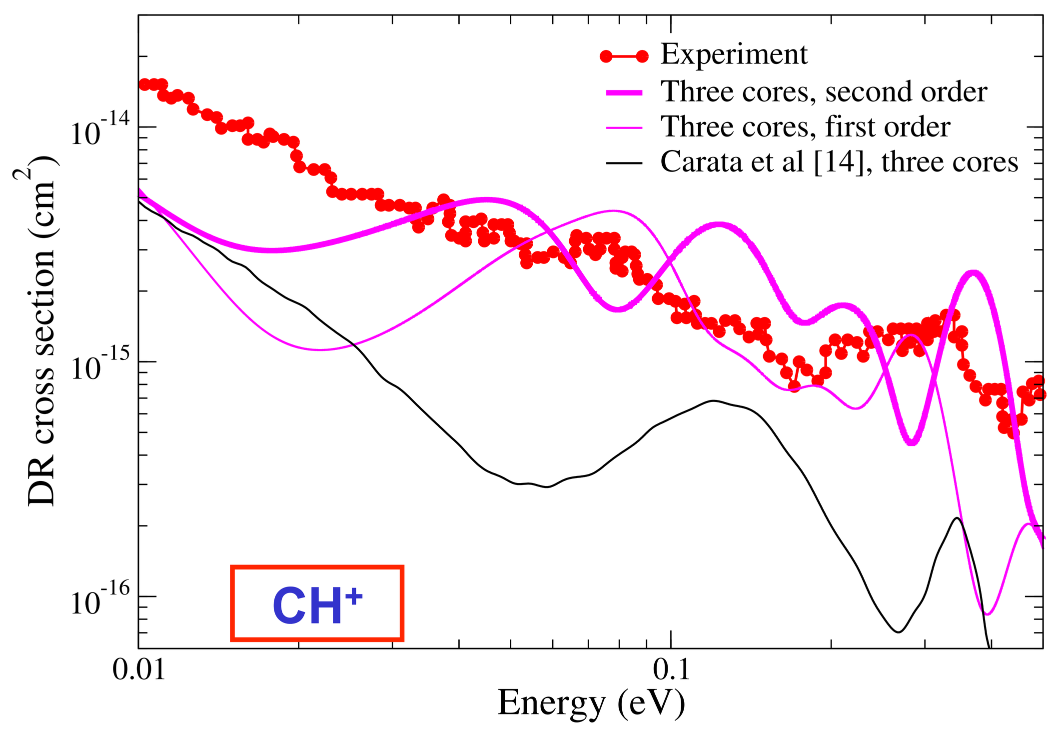

Figure 7.: DR cross sections for CH^+ including two excited cores, compared with TSR storage ring measurements [14] and previous calculations [15].

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ACKNOWLEDGEMENTS

We warmly acknowledge Région Haute-Normandie, the LabEx EMC³, FR-FCM-ITER and USPC-ENUMPP.