ELECTRON-INDUCED EXCITATION AND RECOMBINATION OF BeH+ AND ITS ISOTOPOLOGUES: REACTIONAL DYNAMICS AND RATE COEFFICIENTS

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INTRODUCTION

Among the main elementary processes in cold plasma we find:
Dissociative Recombination **(DR):**

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

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

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

The Multichannel Quantum Defect Theory (MQDT) [1,2] has been employed in computing cross sections and Maxwell rate coefficients for electron-driven reactions involving molecular cations. The key challenge in the use of beryllium as main chamber material for experimental and commercial fusion devices is to understand, predict and control the characteristics of the thermonuclear burning plasma, the plasma edge regimes that result in acceptable erosion performance and the divertor plasma (heat and particle exhaust, impurity control, lifetime).
Due the low mass ratio between beryllium and the D, T plasma fuel ions, beryllium erodes rather easily under plasma exposure by physical and chemical sputtering, a process which releases Be, Be+, and other impurities into the plasma. Significant fractions of the eroded beryllium will be transported towards the divertor and will form compounds with the fuel atoms, molecules and/or molecular ions. In this poster we want to report data on the processes DR, VE, VdE that have been published [4,5,6,7] regarding the impact of the electron with molecular cation of beryllium hydride and its isotopologues.

RESULTS

For the fusion plasma edge, extensive cross sections and rate coefficients have been produced for **BeH^+** (Figure 1, Figure 2), **BeD^+**, **BeT^+** ([3,4,5,6] (Figure3-5).

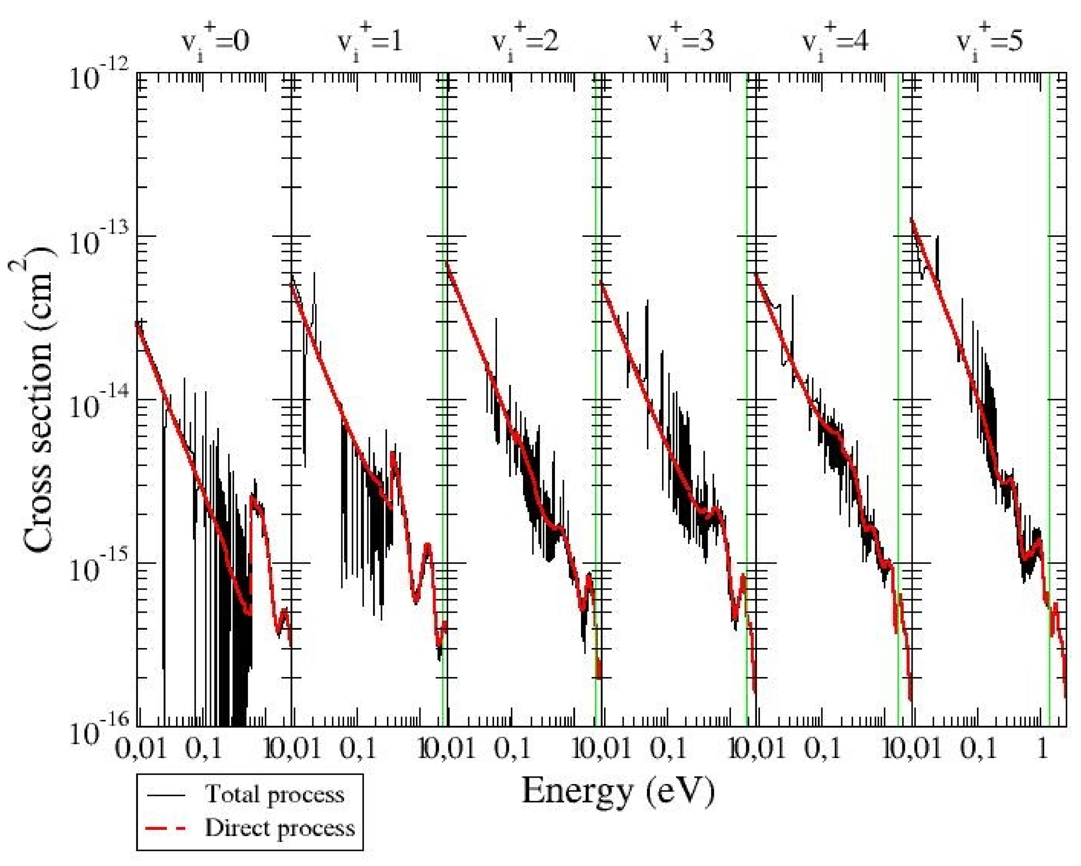

Figure 1. Dissociative recombination cross sections of BeH+ in its electronic ground state and on its lowest vibrational levels, v_i^+, [3]. The numbers label the initial vibrational state of the target.

In view of the simple use of the rate coefficients, the large amount of data obtained for whole processes have been fitted by using the modified Arrhenius type formulas, with the electron temperature range 100 K < T_e < 5000 K. The set of coefficients can be found in the papers mentioned above.

$$k^{fitt}(T) = A\,T^{\alpha} \exp\left[-\frac{B}{T}\right]$$

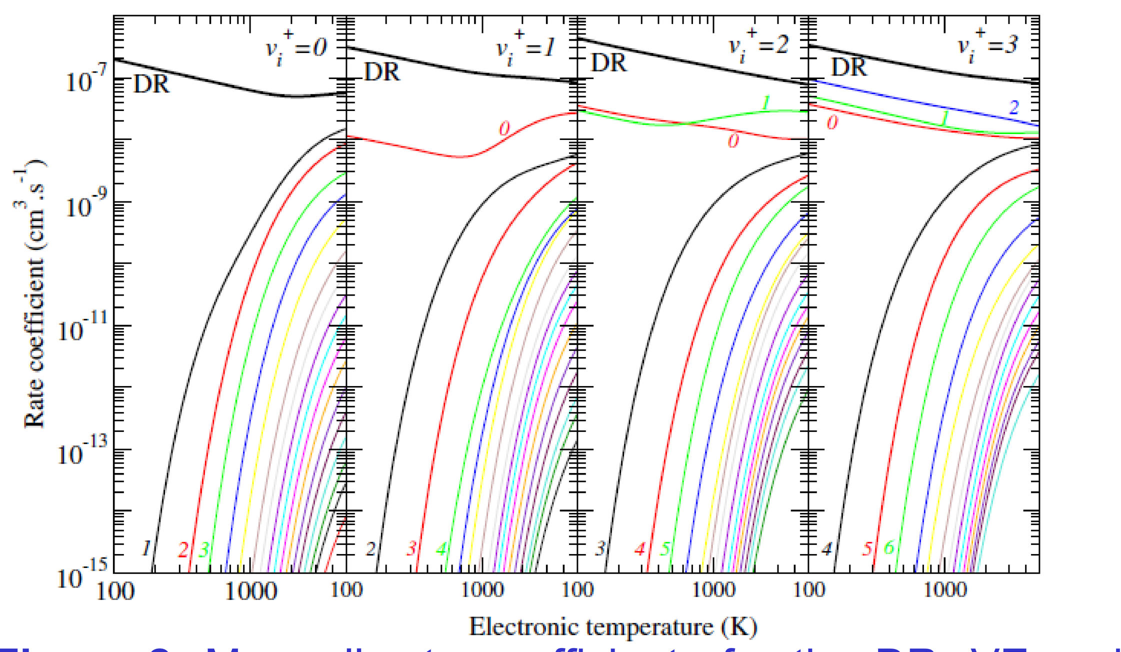

Figure 2. Maxwell rate coefficients for the DR, VE and VdE of BeH^+ ion in its electronic ground state and on its initial vibrational states v_i^+ [3].

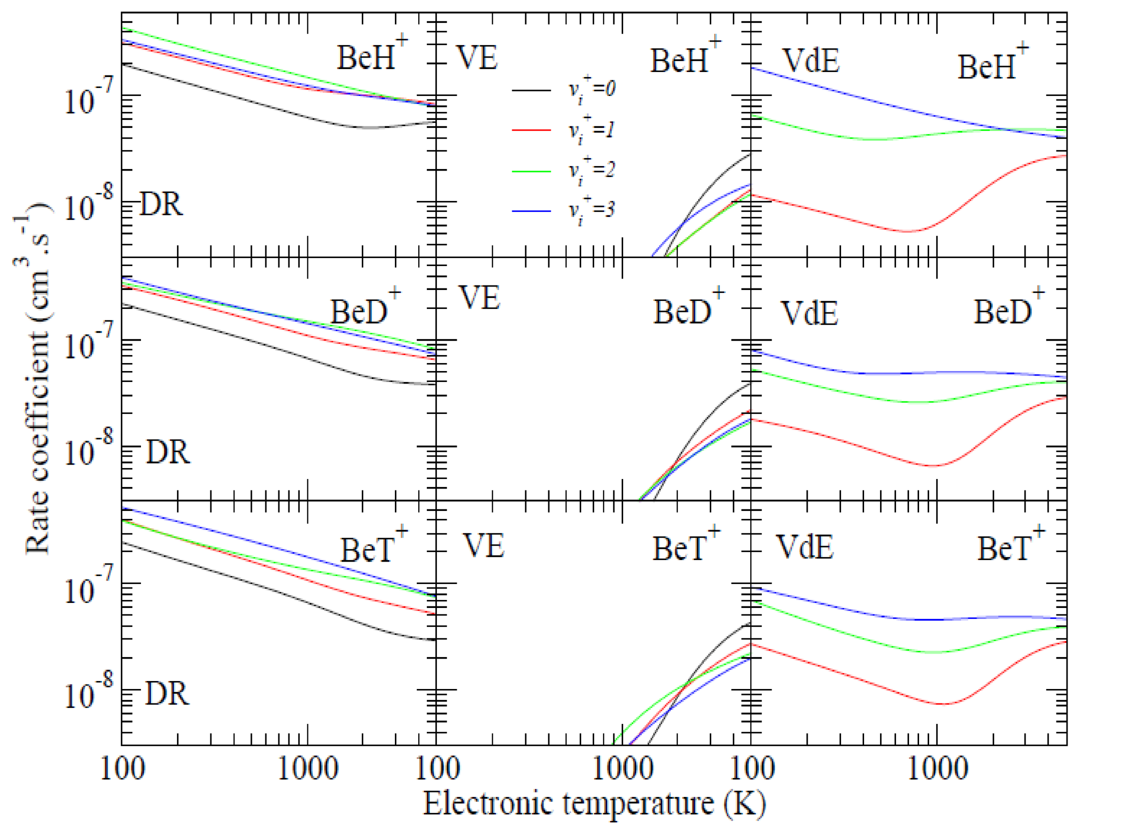

Figure 3. Comparison of Maxwell isotropic rate coefficients for the DR and state-to-state VE and VdE of BeH^+, BeD^+ and BeT^+ [5].

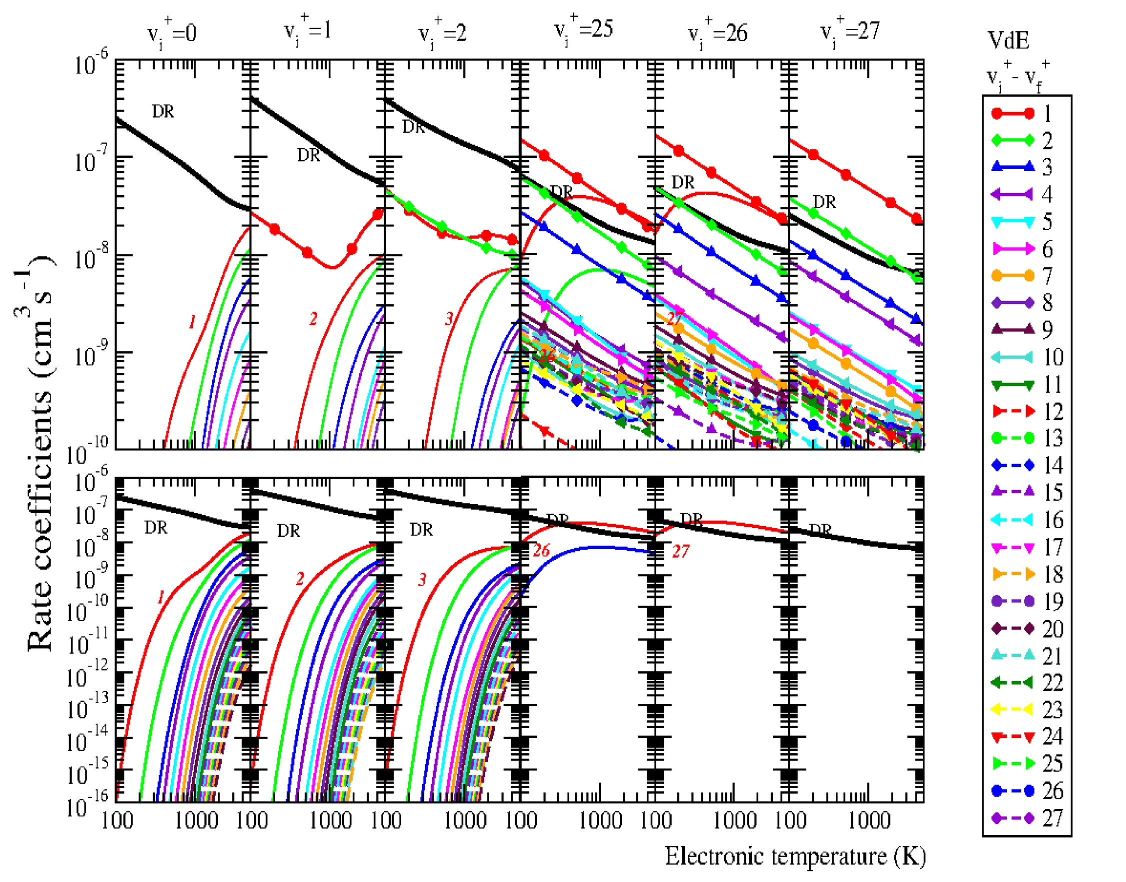

Figure 4. Dissociative Recombination (DR) and state-to-state Vibrational Excitation (VE)/ Vibrational De-Excitation (VdE) rate coefficients of BeT^+ in its ground electronic state.

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Figures 2-4 illustrate quantitatively the competition between the vibrational transitions and dissociative recombination. The energy of the electron is inferior to 2.7eV, value that corresponds to the dissociation threshold of the ground state of the ion. The electron temperature range is 100–5000K.
These rate coefficients strongly depend on the initial vibrational level of the molecular ion.
Studies upon the isotopic effects were also made and presented in Figure 5.

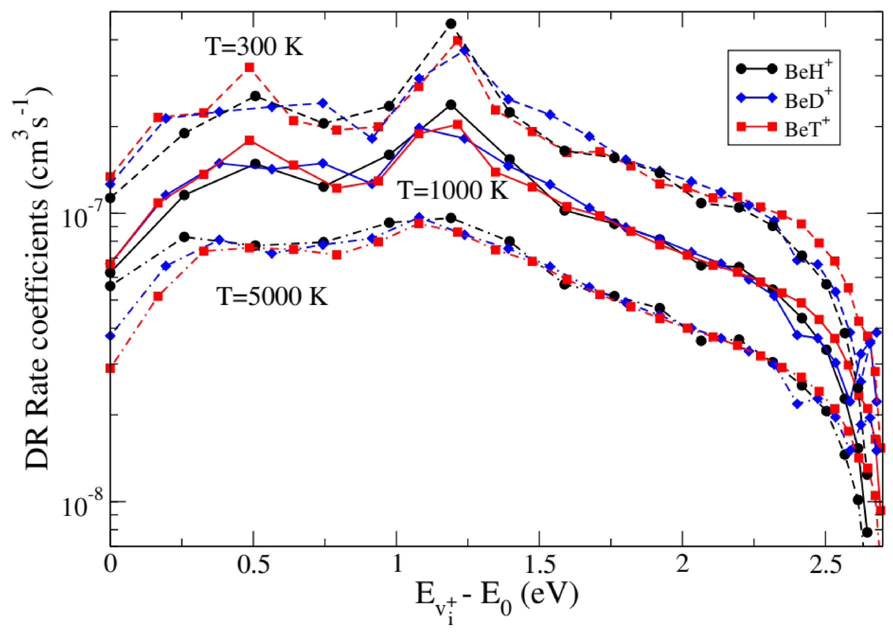

Figure 5. Isotopic effects: Dissociative recombination rate coefficient of the BeH+ (black), BeD+ (blue) and BeT+ (red) molecular cations as function of the energy of the initial vibrational level of the target relative to the ground vibrational level, for three electron temperatures.

CONCLUSIONS

The resulting data are useful in magnetic confinement fusion edge plasma modelling and spectroscopy, in devices with beryllium based main chamber materials, such as the International Thermonuclear Experimental Reactor (ITER) and the Joint European Torus (JET). BeH as well as BeD and BeT molecules are expected to appear in a significant (spectroscopically detectable) amount in the edge and divertor plasmas.

REFERENCES

[1] Ch. Jungen, Handbook of High Resolution Spectroscopy, Wiley & Sons, (2011) 471.

[2] I. F. Schneider, O. Dulieu, J. Robert, Proceedings of DR2013: The 9th International Conference on Dissociative Recombination: Theory, Experiment and Applications, Paris, July 7-12, 2013, EPJ Web of Conferences 84 (2015).

[3] S.Niyonzima, F. Lique, K. Chakrabarti, A. Larson, A. E Orel et I. F. Schneider, "Multichannel-quantum-defect-theory treatment of reactive collisions between electrons and BeH+", Phys. Rev.A 87 (2013) 022713.

[4] S. Niyonzima, S. Ilie, N. Pop, et al., Atomic Data and Nuclear Data Table, 115-116, 287-308 (2017).

[5] S Niyonzima, N Pop, F Iacob, Å Larson, A E Orel, J Zs Mezei, K Chakrabarti, V Laporta , K Hassouni, D Benredjem, A Bultel, J Tennyson , D Reiter and I F Schneider, *Plasma Sources Sci. Technol.* **27,** 025015 (2018).

[6] N. Pop, Iacob, S Niyonzima, A Abdoulanziz, V Laporta, D Reiter, IF Schneider, J Zs Mezei, Atomic Data and Nuclear Data Table, 139, 101414 (2021).

[7] Pop N., Iacob F., et al. Recombination and excitation of molecular cations with electrons: Application to BeD+ and BeT+. AIP Conference Proceedings, 2019, 2071 (1), 020007.