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# DISSOCIATIVE RECOMBINATION OF $BeH^+$ IN THE INTERSTELLAR MEDIUM

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**Abstract.** We report a theoretical study of dissociative recombination (DR) of $BeH^+$ by low energy electron impact, using previously computed molecular data as input for a Multichannel Quantum Defect Theory (MQDT) approach. Three electronic symmetries of BeH, $^2\Pi$, $^2\Sigma^+$, and $^2\Delta$ have been included in the calculations. We present cross sections and thermal rate coefficients ready to be used in the modelling of the $BeH^+$ abundance in the interstellar medium and stellar atmosphere.

## 1 Introduction

Hydride molecules have been observed in many astrophysical media. BeH and its associated ion $BeH^+$ have been identified in stars – including Sun – and comets (Wilkinson *et al.* 1963; Singh 1988; Sauval *et al.* 1984; Shanmugavel *et al.* 2006). The determination of physical and chemical conditions of these media requires the knowledge of the elementary processes relevant for the abundances of these molecules. $BeH^+$ can be destroyed by Dissociative Recombination (DR):

$$BeH^+ + e^-(\varepsilon) \longrightarrow [Be + H](\epsilon)$$

where $\varepsilon$ and $\epsilon$ stand for the incident electron energy and the relative kinetic energy release of the two neutral atoms Be and H, respectively. Unfortunatly, due to the high toxicity of Beryllium, no measurement of the DR rate coefficient of $BeH^+$

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is available. Thus, these data can only be obtained using theory. Theoretical predictions have been performed recently by Roos *et al.* (2009) using a time dependent approach. However, the wave packet technique may not be the most suitable approach at low collision energies of astrophysical interest because of the difficulties of incorporating the indirect mechanism through electronic capture into bound Rydberg states. Here we have employed the molecular data of Roos *et al.* (2009) in a new series of calculations relying on a MQDT-based method (Giusti 1980; Schneider *et al.* 2000). We present the calculations of DR cross sections/rate coefficients at low and intermediate energies/temperatures. These rate coefficients will help in the modelling of various ionized media containing $BeH^+$.

## 2 Molecular data and dissociative recombination calculations

The molecular data consisting of potential energy curves and autoionization widths have previously been computed (Roos *et al.* 2009) by combining electron scattering calculations with structure calculations. By performing multi-reference configuration interaction calculations, adiabatic potential energy curves have been obtained for the ground state of $BeH^+$ and for the excited states of BeH within the relevant symmetries. The potential energy curves and autoionization widths of the resonant states have been obtained using electron scattering calculations. By following the configurations of the resonant states the quasidiabatic potential energy curves and couplings relevant for DR were determined by an orthogonal transformation of the adiabatic states. The dissociative recombination calculations were performed using the MQDT -based method founded by Giusti (1980).

## 3 Results

### *3.1 Cross sections*

We assume that $BeH^+$ is initially in its ground state ($X^1\Sigma^+, v_i^+ = 0$). Using the molecular data invoked above, we have performed a series of MQDT calculations of DR cross sections, exploring for the energy range of the incident electron in the interval 0 – 2.7 eV, which corresponds to a total energy of the system below the dissociation limit of the ground electronic state of $BeH^+$.

In Figure 1 we show the *direct* cross section – obtained by *neglecting* the capture into Rydberg states – namely the contributions of the relevant symmetries, and the global result, after their summation. The $^2\Pi$ symmetry dominates the process at low energy because the potential energy curves of the first and second dissociative states of this symmetry cross the ion potential curve near the equilibrium internuclear distance. Figure 2 displays the DR cross section within the direct and *total* mechanism (*i.e.* including the *indirect* capture through bound Rydberg states). We notice the sudden increase of the global cross section at 0.6 eV, due to the opening of the $^2\Delta$ channel.

The total cross section is characterized by a rich resonant structure, but the resonances play a little role when the cross section is averaged to obtain a rate coefficient.

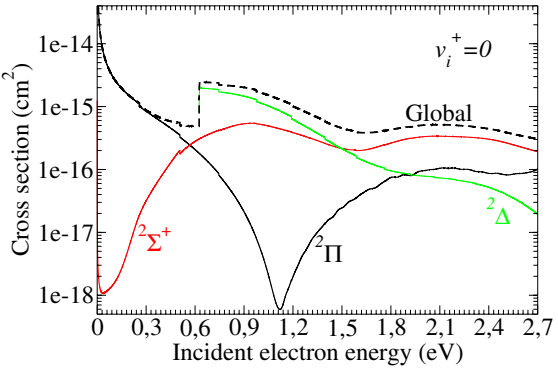


**Fig. 1.** Contribution of each relevant symmetry to the direct DR cross section of $BeH^+$ in its ground state. The dashed line represents the direct cross sections summed over all the electronic states.

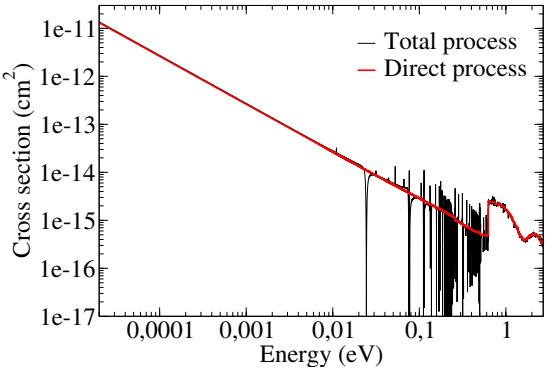


**Fig. 2.** Direct (red thick line) and total (oscillating black thin line) DR cross sections of $BeH^+$ in its ground state.

### *3.2 Rate coefficients*

In order to provide ready-to-use data for the kinetic modelling, we have converted the cross sections into thermal rate coefficients by convoluting the cross section with an isotropic Maxwellian distribution of electron velocities. Figure 3 displays the thermal rate coefficients for DR. The previous DR result obtained by Roos *et al.* (2009) is shown too, but it is restricted to temperatures above 500 K. Indeed, the way the Rydberg states were included within the wave packet approach does not allow for a complete account of the resonances, and this implies a visible difference between the two types of results, notably increasing towards low temperatures. We also show in Figure 3 the rate coefficients corresponding to vibrational excitation (VE) of $BeH^+$ [ $BeH^+(v_i^+) + e^-(\varepsilon) \rightarrow BeH^+(v_f^+) + e^-$]. One can see that the inelastic process is slower than DR in the temperature range considered in this work.

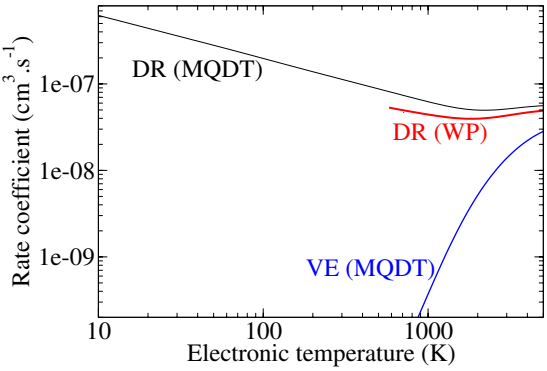


**Fig. 3.** Comparison between MQDT and WP (Ross *et al.* 2009) total DR rate coefficients of $BeH^+$ in its ground state. The MQDT-computed rate coefficient for total VE of $BeH^+$ from its ground state into all the vibrational excited states is also presented.

## 4 Conclusions

Our MQDT computations of the dissociative recombination cross section, valid down to zero energy of the incident electron, complete the previous wave-packet calculations (Roos *et al.* 2009) and support them at intermediate energies. The thermal rate coefficient is computed in the temperature range 10–5000 K and displays an anti-Arrhenius temperature dependence, *i.e.* decreasing magnitude with increasing temperature. More extensive calculations will be performed in order to provide further input data for the kinetic modelling of media of astrophysical and planetary interest.

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