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Charge exchange between bare beryllium and boron with metastable hydrogen atoms at low energies

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Theoretical results for $^{9}Be^{4+}$-H(2*s*) and $^{11}B^{5+}$-H(2*s*) partial and total charge-exchange cross sections at low relative velocities (0.027–0.32 a.u.) are given, using the Landau-Zener method. The necessary molecular parameters for this method are obtained from the exact one-electron diatomic molecule (OEDM) molecular energies. The partial cross sections which are mainly populated are those corresponding to the principal quantum number of separated atoms $n=5$ for Be^{3+} and $n=6$ for B^{4+}. The total cross sections show a rather strong increase with increasing collision energies and a quite large maximum. They lie between the cross sections corresponding to the neighbor reactions for the incident nuclei with $Z=3$ (Li), $Z=6$ (C), and $Z=7$ (N). The atomic collisions with beryllium are very important in plasma tokamaks.

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I. INTRODUCTION

Charge-exchange collisions between bare ions and the ground-state H atoms have been the subject of a rather large amount of work (Gilbody [1] and references therein).

With respect to collisions with "metastable" hydrogen, Blanco, Falcón, and Piacentini [2] considered H^+ as incident ions; Blanco *et al.* [3] He^{2+}; Casaubon and Piacentini [4] Li^{3+}, and Salop [5] C^{6+} and N^{7+}.

In the present work we have completed the systematic up to $Z=7$, studying theoretically the collisions $^{9}Be^{4+}$-H(2*s*) and $^{11}B^{5+}$-H(2*s*). The Landau-Zener (LZ) multicrossing method has been employed as in [5], considering two crossings in each reaction channels.

II. THEORY

A. Be^{4+}-H(2*s*)

The molecular-energy curves were obtained employing the program OEDM developed by Salin [6]. The separated-atom state corresponding to a molecular description of the collision is

$$\psi_{2s}=2^{-1/2}\{\langle 9k\sigma|+\langle 8i\sigma|\} . \tag{1}$$

There are two channels coupled to these initial states:

$$\alpha:\ 9k\sigma\rightarrow 8j\sigma\rightarrow 7i\sigma\rightarrow 6h\sigma\rightarrow 5g\sigma\rightarrow 3d\sigma ,$$

$$\beta:\ 8i\sigma\rightarrow 7h\sigma\rightarrow 6g\sigma\rightarrow 5f\sigma\rightarrow 4d\sigma\rightarrow 3p\sigma .$$

We assume that the crossing $9k\sigma\rightarrow 8j\sigma\rightarrow 7i\sigma$ and $8i\sigma\rightarrow 7h\sigma\rightarrow 6g\sigma$ are totally diabatic, and $5g\sigma\rightarrow 3d\sigma$ and $4d\sigma\rightarrow 3p\sigma$ are totally adiabatic, since the first ones have a small energy difference and the latter ones, on the contrary, are well separated.

Consequently, we have four crossings to be considered, two for each channel (see Figs. 1 and 2):

$$\alpha:\ 7i\sigma\xrightarrow{\alpha_5}6h\sigma\xrightarrow{\alpha_4}5g\sigma ,$$

$$\beta:\ 6g\sigma\xrightarrow{\beta_5}5f\sigma\xrightarrow{\beta_4}4d\sigma ,$$

where each crossing is characterized by the symbol α_n or β_n, with $n=4,5$ depending on the principal quantum number of the final state of the separate atom.

The partial cross section for charge exchange is (see Salop [5])

$$Q_n=(Q_{\alpha_n}+Q_{\beta_n})/2 , \tag{2}$$

where

$$Q_{\gamma_n}=2\pi\int_0^{b_{\gamma_n}}P_{\gamma_n}(b)b\,db , \tag{3}$$

with

$$\gamma=\alpha \text{ or } \beta .$$

$b_{\gamma_n}=R_{c\gamma_n}(1-U_{\gamma_n}/E_0)^{1/2}$ is the maximum impact parameter b for which $R_{c\gamma_n}$ (the internuclear distance R at

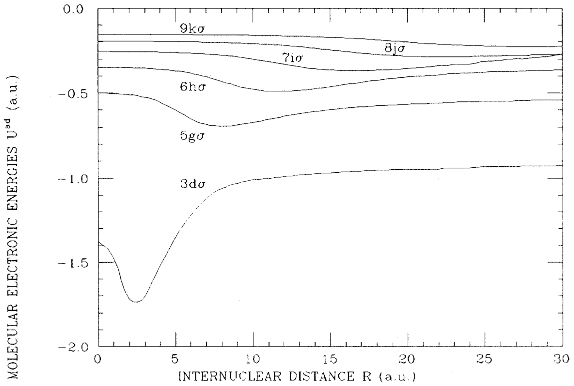

FIG. 1. Molecular electronic energies corresponding to the reaction channel α, for $(BeH)^{4+}$.

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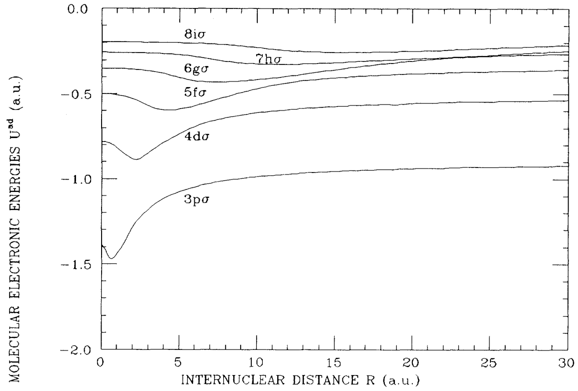

FIG. 2. Molecular electronic energies corresponding to the reaction channel β, for $(\mathrm{BeH})^{4+}$.

the crossing) is reached in the closest approach of nuclei [$dR/dt=0$; see below Eq. (9)]. U_{γ_n} is the diabatic potential energy (including nuclear repulsion) at the crossing, and E_0 is the relative incident energy. The total cross section is directly the sum of the contributions:

$$Q=\sum_n Q_n \; . \tag{4}$$

For the case in which the projectile penetrates the two crossings, we obtain

$$P_{\gamma_5}=p_1(1-p_1)+p_2^2(1-p_1)p_1+p_1(1-p_2)^2(1-p_1) \; , \tag{5}$$

$$P_{\gamma_4}=2p_2(1-p_1)(1-p_2) \; , \tag{6}$$

where p_i is the well-known LZ probability, for each crossing, of remaining in the same diabatic state when the projectile passes through a crossing:

$$p=\{-\pi(\Delta U^{\mathrm{ad}})^2/(2v_r D)\} \; , \tag{7}$$

where ΔU^{ad} is the difference of adiabatic energies at the crossing point,

$$D=d(U-U')/dR\,|_{R_c} \; , \tag{8}$$

where $(U-U')$ is the difference between diabatic potential energies involved in the crossing, and

$$v_r=dR/dt=v_0\sqrt{1-U/E_0-(b/R_c)^2} \tag{9}$$

is the radial velocity at the crossing (result emerging from the classical movement of nuclei), v_0 is the impact velocity.

If the particle does not penetrate the $R_{c\gamma_4}$ crossing, then P_{γ_5} is reduced to the simple equation used in LZ for only one crossing:

$$P_{\gamma_5}=2p_1(1-p_1) \; .$$

The molecular parameters are presented in Table I. With

TABLE I. Molecular parameters corresponding to the Be^{4+}-$\mathrm{H}(2s)$ system in the crossings α_5, α_4, β_5, and β_4, in atomic units.

Parameter	Channel α_5	α_4	β_5	β_4
R_c	21.5	13.5	12	6.4
ΔU^{ad}	0.04	0.12	0.04	0.11
D	0.02	0.048	0.02	0.071
U	−0.183	−0.243	−0.08	0.015

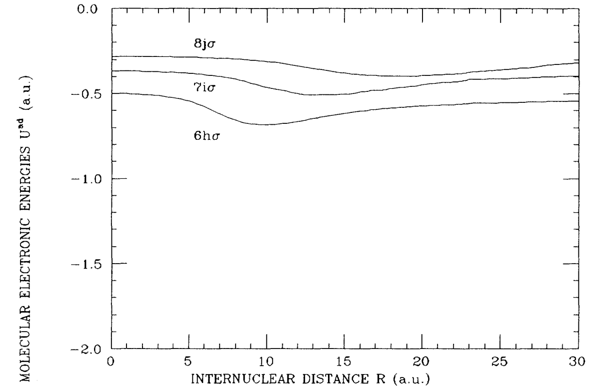

FIG. 3. Molecular electronic energies corresponding to the reaction channel α, for $(\mathrm{BH})^{5+}$.

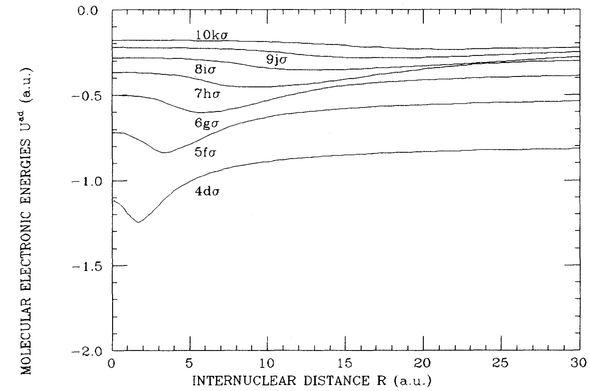

FIG. 4. Molecular electronic energies corresponding to the reaction channel β, for $(\mathrm{BH})^{5+}$.

TABLE II. Molecular parameters corresponding to the B^{5+}-$\mathrm{H}(2s)$ system in the crossings α_6, α_5, β_6, and β_5, in atomic units.

Parameter	Channel α_6	α_5	β_6	β_5
R_c	22	16	14.5	9.5
ΔU^{ad}	0.04	0.11	0.03	0.09
D	0.02	0.04	0.016	0.036
U	−0.172	−0.237	−0.085	−0.063

them we can obtain partial and total cross sections (Table III).

B. B^{5+}-H(2s)

In this case the entrance channels are $11m\sigma$ and $10k\sigma$ and the molecular "cascades" result:

$$\alpha:\ 11m\sigma\rightarrow 10l\sigma\rightarrow 9k\sigma\rightarrow 8j\sigma\rightarrow 7i\sigma\rightarrow 6h\sigma\rightarrow 4f\sigma\ ,$$

$$\beta:\ 10k\sigma\rightarrow 9j\sigma\rightarrow 8i\sigma\rightarrow 7h\sigma\rightarrow 6g\sigma\rightarrow 5f\sigma\rightarrow 4d\sigma\ .$$

The diabatic crossings are $11m\sigma\rightarrow 10l\sigma\rightarrow 9k\sigma\rightarrow 8j\sigma$ and $10k\sigma\rightarrow 9j\sigma\rightarrow 8i\sigma\rightarrow 7h\sigma$, and the diabatic ones are $6h\sigma\rightarrow 4f\sigma$ and $5f\sigma\rightarrow 4d\sigma$.

Then the transitions take place at two crossings for each channel (see Figs. 3 and 4):

$$\alpha:\ 8j\sigma\xrightarrow{\alpha_6} 7i\sigma\xrightarrow{\alpha_5} 6h\sigma\ ,$$

$$\beta:\ 7h\sigma\xrightarrow{\beta_6} 6g\sigma\xrightarrow{\beta_5} 5f\sigma\ .$$

In a similar way to the case of beryllium we show the molecular parameters in Table II. With them we can obtain partial and total cross sections (Table III).

III. RESULTS

In Table III we can see the relative contributions to the charge-exchange cross sections of each channel and principal quantum number. In general, in the energy range considered in the present work, for both reactions $^9Be^{4+}$-H(2s) and $^{11}B^{5+}$-H(2s) the outermost crossings collaborate to a greater extent.

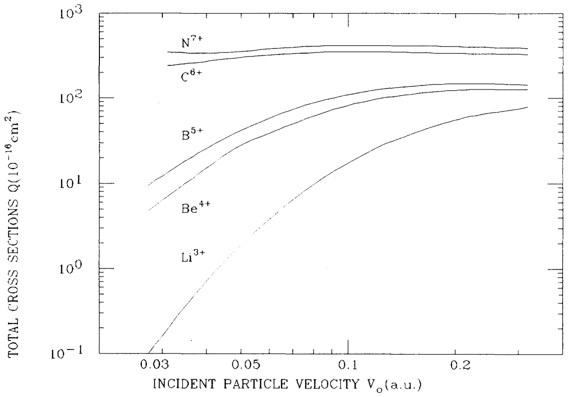

FIG. 5. Charge-exchange total cross sections for $^9Be^{4+}$-H(2s) and $^{11}B^{5+}$-H(2s) (present work); Li^{3+}-H(2s) by Casaubon and Piacentini [4] and C^{6+},N^{7+}-H(2s) by Salop [5]. (All are theoretical results.)

Consequently the principal quantum number which is most populated by electron capture is the larger of the two included in the treatment ($n=5$ for Be^{3+} and $n=6$ for B^{4+}).

It must be pointed out that following Salop [5] the resonance channels giving rise to Be^{3+} ($n=8$) and B^{4+} ($n=10$) were not included in the present study, since these reactions are more asymmetric than those with H^+ and He^{2+} as incident particles, where the contributions of the resonance channels cannot be neglected (Blanco, Falcón, and Piacentini [3]).

TABLE III. Charge-exchange cross sections corresponding to each channel γ_n, the partial Q_n and the total Q contributions (units of 10^{-16} cm^2) as a function of the incident particle velocity.

	$Be^{4+}+H(2s)$						
V_0 (a.u.)	$\frac{1}{2}Q_{\alpha_5}$	$\frac{1}{2}Q_{\alpha_4}$	$\frac{1}{2}Q_{\beta_5}$	$\frac{1}{2}Q_{\beta_4}$	Q_5	Q_4	Q
0.319	83.68	12.91	26.78	2.816	110.46	15.73	126.19
0.229	81.18	16.16	26.00	3.528	107.18	19.69	126.87
0.183	75.68	17.56	24.19	3.829	99.87	21.39	121.26
0.137	64.32	17.71	20.42	3.833	84.74	21.54	106.28
0.0914	43.21	14.30	13.42	2.994	56.63	17.29	73.92
0.0639	24.65	9.185	7.337	1.763	31.99	10.95	42.94
0.0457	11.84	4.851	5.004	0.763	16.84	5.614	22.45
0.0366	6.549	2.876	1.619	0.350	8.168	3.226	11.39
0.0274	2.757	1.365	0.542	0.091	3.299	1.456	4.76
	$B^{5+}+H(2s)$						
V_0 (a.u.)	$\frac{1}{2}Q_{\alpha_6}$	$\frac{1}{2}Q_{\alpha_5}$	$\frac{1}{2}Q_{\beta_6}$	$\frac{1}{2}Q_{\beta_5}$	Q_6	Q_5	Q
0.319	84.47	18.85	36.04	4.575	120.51	23.42	143.93
0.229	81.80	23.42	37.69	6.335	119.49	29.75	149.24
0.183	76.32	25.38	37.36	7.485	113.68	32.86	146.54
0.137	65.09	25.38	34.92	8.571	100.01	33.95	133.96
0.0914	44.04	20.31	27.88	8.602	71.92	28.91	100.83
0.0639	25.25	12.93	19.36	6.867	44.61	19.79	64.41
0.0457	12.09	6.756	11.47	4.380	23.56	11.13	34.69
0.0366	6.621	3.966	7.243	2.818	13.86	6.78	20.64
0.0274	2.718	1.848	3.460	1.327	6.178	3.175	9.353

From Table III and the comparison with other reactions made in Fig. 5 we can see that the total charge-exchange cross sections show a rather strong increase with increasing energy and arrive at a quite large value at the end of the energy range (around $v_0 = 0.2-0.25$ a.u.). Also they lie between the neighbor reactions for the incident nuclei with $Z = 3$ (Li), $Z = 6$ (C), and $Z = 7$ (N).

As a test of the isotopic effects we have calculated the LZ cross sections for $^{8}Be^{4+}$ and $^{10}B^{5+}$ in collision with $H(2s)$. In the lower (more sensitive) energy range the relative differences with the results shown in Table III for Q are no greater than 10%.

In the present work we have completed the theoretical study of reactions between low-nuclear-charge bare ions ($Z \leq 7$) and metastable hydrogen. It will be welcome to have experimental data on these interesting systems.

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[1] H. B. Gilbody, Phys. Scr. **23**, 143 (1981).
[2] S. A. Blanco, C. A. Falcón, and R. D. Piacentini, J. Phys. B **19**, 3945 (1986).
[3] S. A. Blanco, C. A. Falcón, C. O. Reinhold, J. I. Casaubon, and R. D. Piacentini, J. Phys. B **20**, 6295 (1987).
[4] J. I. Casaubon and R. D. Piacentini, J. Phys. B **17**, 1623 (1984).
[5] A. Salop, Phys. Rev. A **13**, 1321 (1976).
[6] A. Salin, Comput. Phys. Commun. **14**, 121 (1978); **20**, 462 (1978).