CALCULATIONS OF CHARGE TRANSFER AND IONISATION CROSS SECTIONS FOR ION-H_2(D_2,DT, T_2) COLLISIONS

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1 INTRODUCTION

Charge transfer cross sections in collisions of multicharged ions with molecules are of interest in the outer regions of the plasma in fusion devices, particularly near divertors. In this paper we summarize calculated cross sections for collisions of ions with H_2 (also D_2, DT and T_2) for energies above 40 eV/amu.

Our methods are based on the sudden approximation for the treatment of the ro-vibrational motion of the diatom. In some cases, we have used the additional familiar Franck-Condon (FC) approximation and the cross sections have been obtained from calculations at only the target equilibrium distance ρ_0. Partial vibrational cross sections can be obtained by multiplying the FC ones by the FC factors of Table I [1]. At low velocities, we have employed a close-coupling expansion for the electronic wavefunction in terms of *ab initio* molecular functions (see [2]). In each case, the characteristics of the calculation, such as the basis set, were chosen from consideration of the energy and coupling diagrams [2]–[9]. At high impact energies (9–625 keV/amu for charge transfer and 9 keV/amu–2.5 MeV/amu for ionisation) classical trajectory calculations have been carried out [3].

Comparison with experimental results and other calculations (not shown here) are included in the published papers [2]–[9].

Cross sections are tabulated as a function of the relative impact velocity, v (in a.u.), and the corresponding energies are $E = 24.982\ v^2$ keV/amu.

2 $H^+ + H_2(X^1\Sigma_g^+, \nu=0,1)$

We have obtained single electron capture (SEC) vibrationally resolved cross section using the sudden approximation. The basis set includes the lowest two states of H_3^+. SEC cross sections from $\nu=0$ and $\nu=1$ of $H_2(X\ ^1\Sigma_g^+)$ are given in Table II and plotted in Figure 1.

State-to-state vibrational cross sections are published in [1], as well as results for D_2, DT, and T_2 targets.

3 $Li^+ + H_2$

A 5-electronic-state calculation for the system LiH_2^+ was performed [1] in the framework of the FC approximation. Orientation averaged cross sections for SEC and excitation to $H_2(B\ ^1\Sigma_u^+)$ are given in Table III and plotted in Figure 2.

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4 $C^{2+}+H_2$

13- and 16- state calculations were performed for the ground ($2s^2;^1S$) and metastable ($2s2p;^3P$) states of C^{2+} respectively. The collinear geometry and the FC approximation were employed [5]. Results are shown in Figure 3 and Table IV. More accurate calculations, using the sudden approximation, have been also carried out for collisions with the metastable projectile [6]. In this case, cross sections to individual vibrational states of H_2^+ have been obtained.

5 $C^{3+}+H_2$

Calculations have been carried out using the FC approximation, collinear geometry and a basis of 8 electronic states. Double electron capture (DEC) leading to Coulomb explosion of the diatom is competitive with SEC and the corresponding cross sections are listed in Table V and plotted in Figure 4. Preliminary results with a smaller basis were published in [7].

6 $C^{4+}+H_2$

Calculations using the sudden approximation and a basis of 8 electronic states were reported in [8]. Our results include state-selected (vibrational and electronic) cross sections in SEC, as well as cross sections for transfer dissociation and vibrational excitation in collisions with H_2, D_2 and DT. We give cross sections for SEC into the main exit electronic channels in Table VI and Figure 5.

7 $N^{5+}+H_2$

A model potential treatment has been used to evaluate the molecular wavefunctions. The Hamiltonian matrix elements between the two-electron wavefunction have been calculated by using the equivalent-electron approximation, as explained in [9]. The dynamical basis includes the entrance channel and 7 SEC channels. Total charge transfer cross sections are given in Table VII and plotted in Figure 6. Preliminary results and comparison with experimental data were reported in [4].

8 CTMC calculations

We have calculated SEC and single ionisation (SI) cross sections for H^+, He^{2+}, Li^{3+}, Be^{4+}, B^{5+}, C^{6+}, N^{7+} and O^{8+} in collisions with H_2, using the improved impact parameter CTMC treatment (see [3]). The calculation employs the FC approximation and a model potential for the H_2 target. Results for SI are plotted in Figure 7 and tabulated in Table VIII. The corresponding SEC results are given in Figure 8 and Table IX. As shown in [3], these cross sections can be used at energies beyond the peak values for collisions of dressed ions with H_2.

Analogously to the ion-atom case, we have obtained scaling laws of the SEC and SI cross sections as functions of the charge q of the projectile and velocity v.

$$\sigma_{\rm SEC}^{\rm scaled}(q, vq^{0.11}) = \sigma_{\rm SEC}(1, v)q \tag{1}$$

$$\sigma_{\rm SI}^{\rm scaled}(q,v) = \sigma_{\rm SI}(1,v) q^{2\left\{0.92-\exp[-0.57(v-0.01q)]-\exp\left[-1.8(v^2-0.08q)\right]\right\}} \tag{2}$$

9 CONCLUDING REMARKS

In the last few years, we have developed new methods to treat ion-H_2 collisions with a similar accuracy to those of ion-atom. These methods have been applied to several ions. We plan to extend our calculations to lower velocities of interest in cold regions of fusion plasma. A more detailed treatment of the anisotropy in the ion-target interaction will also be considered. Calculations involving projectiles in both ground and metastable states are being carried out where experimental uncertainties in the composition of the initial beams exist. Collisions with complex, heteronuclear targets is also planed.

Acknowledgments

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TABLE I: FRANCK-CONDON FACTORS FOR H_2, D_2, DT AND T_2.

ν'	H_2	D_2	DT	T_2
0	0.088088	0.032798	0.023775	0.015375
1	0.163359	0.086461	0.068723	0.049741
2	0.181715	0.129654	0.111744	0.089406
3	0.159648	0.146563	0.135583	0.118563
4	0.123301	0.139736	0.137472	0.130021
5	0.088460	0.119268	0.123728	0.125349
6	0.060893	0.094501	0.102574	0.110319
7	0.041047	0.071197	0.080280	0.090900
8	0.027458	0.051864	0.060352	0.071390
9	0.018389	0.036974	0.044134	0.054148
10	0.012398	0.026026	0.031692	0.040062
11	0.008440	0.018211	0.022508	0.029137
12	0.005807	0.012731	0.015899	0.020957
13	0.004033	0.008925	0.011218	0.014979
14	0.002816	0.006293	0.007932	0.010679
15	0.001961	0.004470	0.005635	0.007618
16	0.001342	0.003204	0.004030	0.005450
17	0.000873	0.002318	0.002905	0.003919
18		0.001693	0.002112	0.002835
19		0.001247	0.001550	0.002067
20		0.000925	0.001147	0.001519
21		0.000689	0.000857	0.001125
22		0.000513	0.000644	0.000841
23		0.000378	0.000486	0.000634
24		0.000273	0.000368	0.000481
25		0.000189	0.000277	0.000368
26			0.000206	0.000282
27			0.000148	0.000217
28				0.000167
29				0.000127

TABLE II: CROSS SECTIONS (IN UNITS OF 10^{-16} cm^2) FOR THE REACTIONS $H^+ + H_2(X\ ^1\Sigma_g^+, \nu = 0, 1) \longrightarrow H + H_2^+(X\ ^2\Sigma_g^+)$.

v(a.u.)	ν=0	ν=1
0.045	0.02	0.19
0.063	0.11	0.64
0.089	0.45	1.68
0.100	0.69	2.20
0.141	2.07	4.47
0.200	4.79	7.00
0.300	8.10	9.24
0.400	8.99	9.15

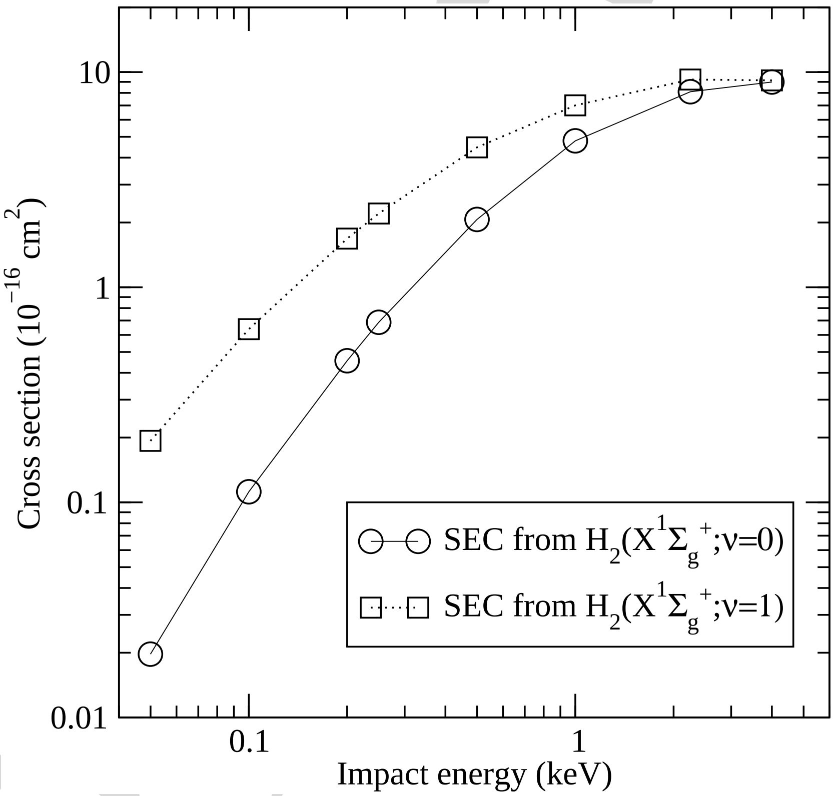

Figure 1: Cross sections for the reactions $H^+ + H_2(X\ ^1\Sigma_g^+; \nu = 0, 1) \longrightarrow H + H_2^+(X\ ^2\Sigma_g^+)$.

TABLE III: CROSS SECTIONS (IN UNITS OF 10^{-16} cm^2) FOR THE SEC REACTIONS $Li^+ + H_2 \longrightarrow Li(2s) + H_2^+$ AND $Li^+ + H_2 \longrightarrow Li(2l) + H_2^+$, AND THE EXCITATION REACTION $Li^+ + H_2(X\ ^1\Sigma_g^+) \longrightarrow Li^+ + H_2(B\ ^1\Sigma_u^+)$.

v(a.u.)	Li(2s)	Li(2l)	$H_2(B\ ^1\Sigma_u^+)$
0.063	0.02	0.03	0.04
0.089	0.04	0.10	0.05
0.100	0.07	0.13	0.06
0.141	0.06	0.21	0.06
0.200	0.18	0.48	0.15
0.250	0.29	0.53	0.23
0.300	0.31	0.63	0.27
0.350	0.31	0.79	0.30
0.400	0.41	0.99	0.29
0.500	0.74	1.46	0.23

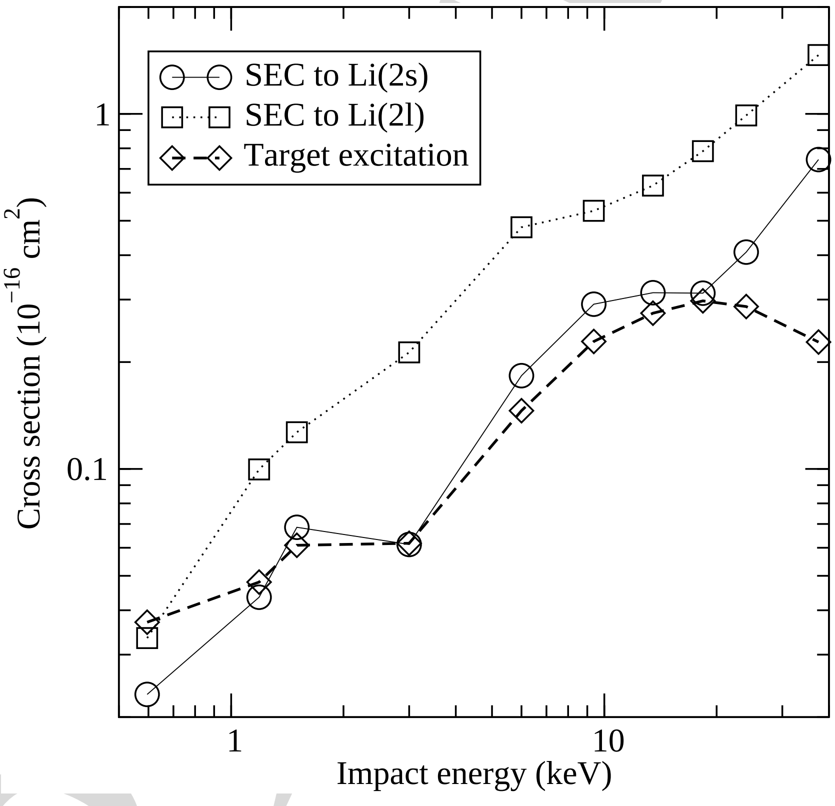

Figure 2: Cross sections for the SEC reactions $Li^+ + H_2 \longrightarrow Li(2s) + H_2^+$ *and* $Li^+ + H_2 \longrightarrow Li(2l) + H_2^+$, *and the excitation reaction* $Li^+ + H_2(X\ ^1\Sigma_g^+) \longrightarrow Li^+ + H_2(B\ ^1\Sigma_u^+)$.

TABLE IV: FC SEC CROSS SECTIONS (IN UNITS OF 10^{-16} cm^2) FOR C^{2+}+H_2(X $^1\Sigma_g^+$) COLLISIONS.

v (a.u.)	$C^{2+}(^1S)$	$C^{2+}(^3P)$
0.045	6.053	17.514
0.048	5.808	18.083
0.052	5.490	18.067
0.055	5.309	18.517
0.058	5.140	18.862
0.060	5.102	18.894
0.080	5.460	19.875
0.100	6.143	19.461
0.115	6.763	18.499
0.120	6.828	18.143
0.140	7.379	16.926
0.160	8.165	16.092
0.180	8.952	15.113
0.200	9.302	13.956
0.220	9.587	12.773
0.240	9.873	11.671
0.260	10.130	10.716

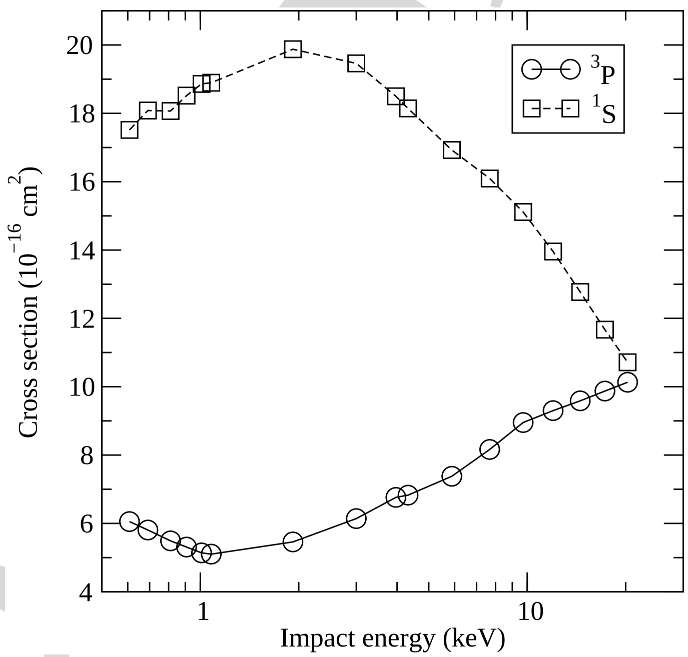

Figure 3: FC cross sections for the reactions $C^{2+}(^1S,^3P)+H_2(X\ ^1\Sigma_g^+, \nu = 0) \longrightarrow C^+ + H_2^+(X\ ^2\Sigma_g^+)$.

TABLE V: FC SEC AND DEC CROSS SECTIONS (IN UNITS OF 10^{-16} cm^2) FOR C^{3+}+H_2 COLLISIONS.

v(a.u.)	SEC	DEC
0.100	7.781	4.518
0.120	6.280	4.832
0.150	5.947	4.785
0.200	6.358	4.407
0.250	6.444	3.972
0.300	6.366	3.694
0.350	6.189	3.548
0.400	5.965	3.470
0.450	5.730	3.423
0.500	5.505	3.391

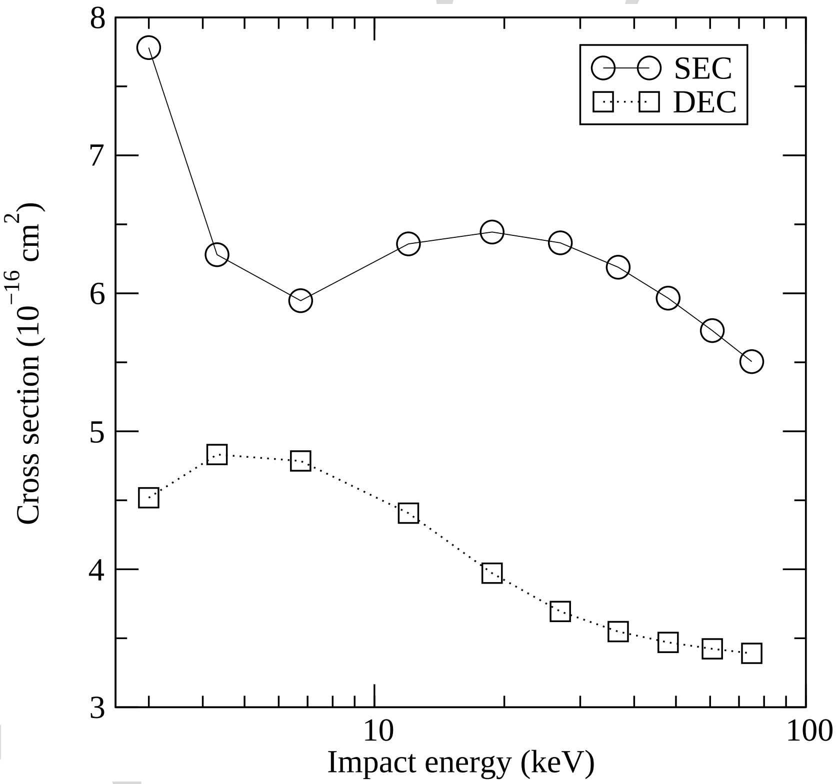

Figure 4: FC SEC and DEC cross sections for the collision C^{3+}+H_2.

TABLE VI: SUDDEN CROSS SECTIONS (IN UNITS OF 10^{-16} cm^2) FOR THE REACTION C^{4+}+H_2⟶C^{3+}(1s^{2}3l)+H_2^+(X $^2\Sigma_g^+$).

v(a.u.)	l=0	l=1	l=2	Total
0.045	16.9	24.7	1.1	42.8
0.060	20.1	20.7	1.1	42.0
0.071	21.4	18.4	1.2	40.9
0.077	21.8	17.7	1.3	40.8
0.089	22.1	17.3	1.7	41.1
0.100	22.1	16.9	2.2	41.3
0.122	22.2	14.9	3.0	40.0
0.141	22.1	12.4	3.7	38.1
0.200	19.9	9.6	3.8	33.3
0.253	17.1	9.8	3.9	30.8
0.300	14.9	9.7	4.4	29.1

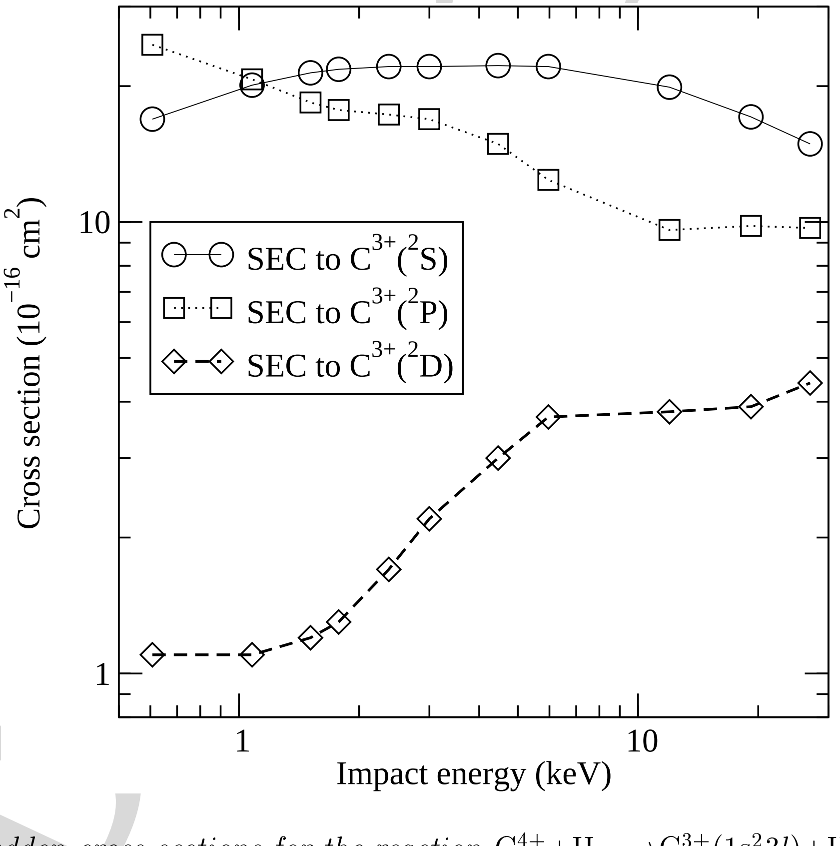

Figure 5: Sudden cross sections for the reaction C^{4+}+H_2⟶C^{3+}(1s^{2}3l)+H_2^+(X $^2\Sigma_g^+$).

TABLE VII: TOTAL CHARGE TRANSFER CROSS SECTIONS (IN UNITS OF 10^{-16} cm^2) FOR THE COLLISION $N^{5+}+H_2$.

v(a.u.)	σ	v(a.u.)	σ
0.0447	1.350	0.320	14.308
0.0632	2.271	0.330	14.819
0.089	3.752	0.340	15.453
0.100	4.250	0.350	16.155
0.125	5.427	0.360	16.864
0.150	6.486	0.370	17.532
0.175	7.623	0.380	18.131
0.200	9.236	0.390	18.662
0.210	9.861	0.400	19.095
0.220	10.380	0.410	19.397
0.230	10.743	0.425	19.610
0.240	11.162	0.440	19.565
0.250	11.680	0.450	19.469
0.260	12.200	0.460	19.370
0.270	12.649	0.500	19.428
0.300	13.656	0.540	20.238
0.310	13.938		

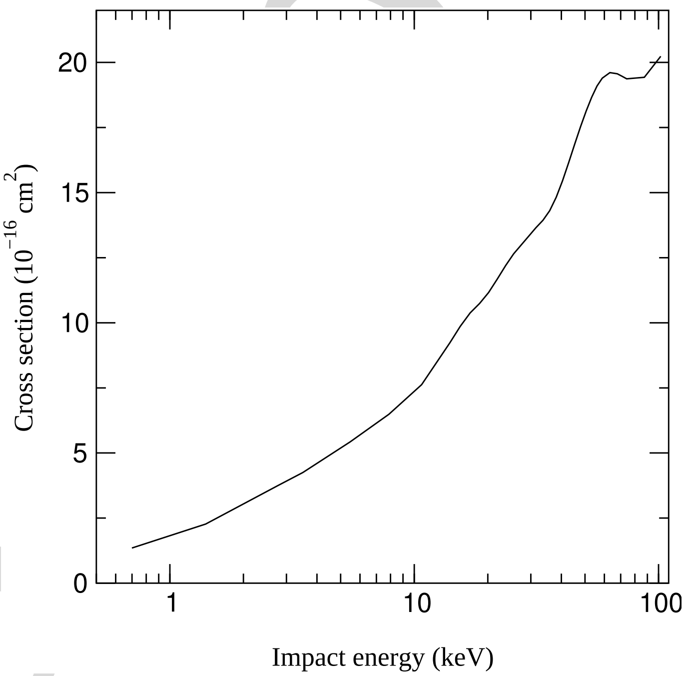

Figure 6: Total charge transfer cross section for the collision $N^{5+}+H_2$.

TABLE VIII: SI CROSS SECTIONS (IN UNITS OF 10^{-16} cm^2) FOR A^{q+}+H_2 COLLISIONS, AS FUNCTIONS OF THE RELATIVE VELOCITY.

v(a.u.)	H^+	He^{2+}	Li^{3+}	Be^{4+}	B^{5+}	C^{6+}	N^{7+}	O^{8+}
0.6	0.235	0.112		0.019				
0.8	0.697	0.405	0.279	0.237	0.164	0.138		
1.0	1.095	1.023	0.877	0.814	0.773	0.684	0.642	0.538
2.0	2.069	5.511	9.036	12.502	15.724	18.893	21.735	24.304
3.0	1.232	3.732	6.549	9.741	13.191	16.697	20.511	24.295
5.0	0.301	1.615	3.119	4.786	6.677	8.750	10.978	13.410
8.0	0.199	0.725	1.486	2.413	3.454	4.613	5.8485	7.163
10.0	0.127	0.488	1.040	1.699	2.475	3.354	4.293	5.282
12.0	0.096	0.368	0.772	1.289	1.874	2.514	3.241	4.044
14.0	0.070	0.292	0.615	1.019	1.487	2.018	2.569	3.212
16.0	0.058	0.214	0.491	0.814	1.195	1.626	2.115	2.615

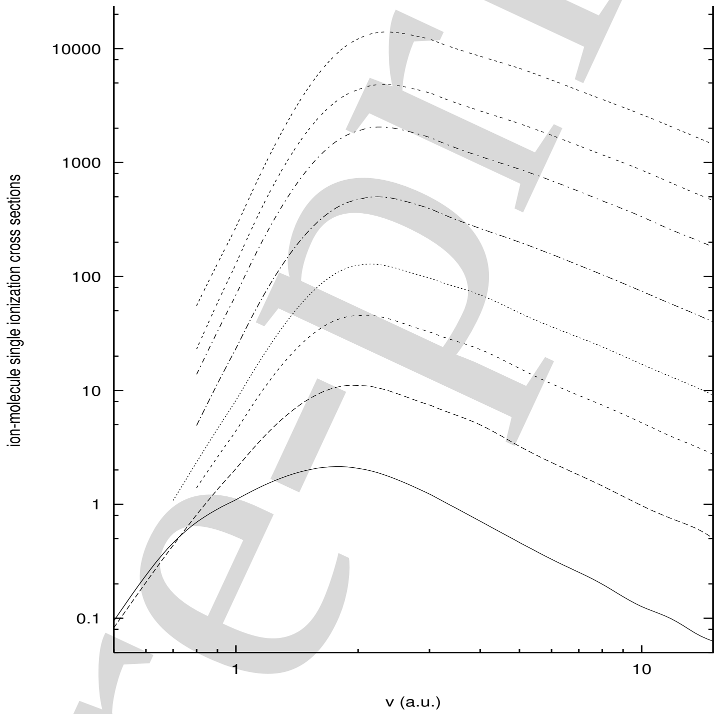

Figure 7: SI cross sections as functions of the relative velocity v, for A^{q+}+H_2 *collisions (in units of 10^{-16} cm^2 and scaled as stated below). From below to above, lines correspond to collisions with different projectiles:* H^+, He^{2+} (data × 2), Li^{3+} (data × 5), Be^{4+} (data × 10), B^{5+} (data × 30), C^{6+} (data × 100), N^{7+} (data × 200), *and* O^{8+} (data × 500).

TABLE IX: SEC CROSS SECTIONS (IN UNITS OF 10^{-16} cm^2) FOR A^{q+}+H_2 COLLISIONS, AS FUNCTIONS OF THE RELATIVE VELOCITY.

v(a.u.)	H^+	He^{2+}	Li^{3+}	Be^{4+}	B^{5+}	C^{6+}	N^{7+}	O^{8+}
0.6	6.451	13.214						
0.8	5.932	12.286	18.396	22.872	29.422	34.684	39.955	45.012
1.0	4.608	10.557	16.251	21.724	27.234	32.679	38.133	43.432
2.0	0.237	0.799	1.491	2.503	3.812	5.210	6.937	8.910
3.0	0.018	0.063	0.133	0.184	0.253	0.341	0.444	0.563
5.0		0.002	0.004	0.004	0.004	0.004	0.005	0.007

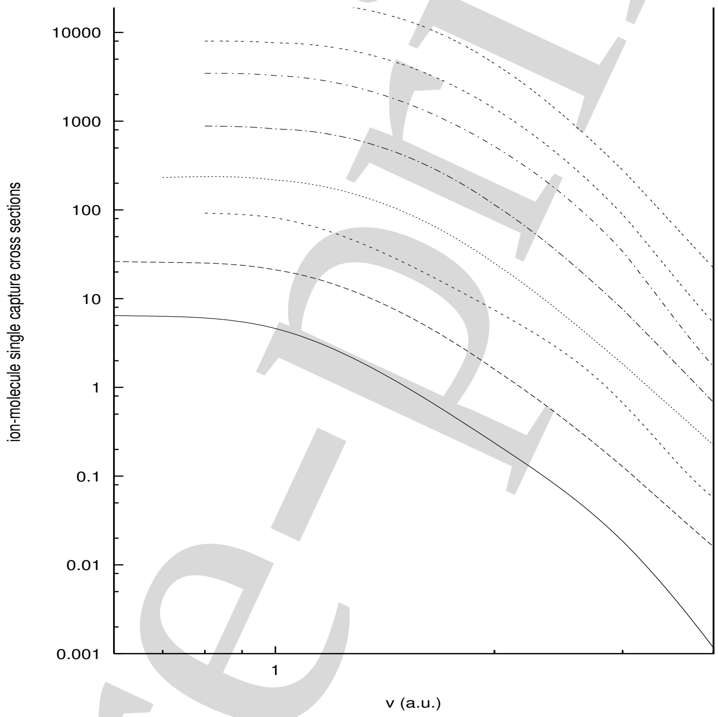

Figure 8: SEC cross sections, as functions of the relative velocity v, for A^{q+}+H_2 *collisions (in units of 10^{-16} cm^2 and scaled as stated below). From below to above, lines correspond to collisions with different projectiles*: H^+, He^{2+} (data × 2), Li^{3+} (data × 5), Be^{4+} (data × 10), B^{5+} (data × 30), C^{6+} (data × 100), N^{7+} (data × 200), *and* O^{8+} (data × 500).