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Intrashell mixing following electron capture from atomic hydrogen targets by slow ions. I — Fully stripped projectiles

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Abstract. — The influence of the Stark effect on the l distribution of excited states produced by electron capture from atomic hydrogen into slow fully stripped ions is studied. The Stark effect is strong enough, in these mono-electronic systems, to preclude any relation between the final l distribution and the primary process of electron capture. The latter determines the m distribution through « geometrical » effects, which supports the utility of measuring the polarization of radiation emitted by decay of the excited states formed in the collision.

1. Introduction.

It is well established both theoretically and experimentally that electron capture by slow multicharged ions from atoms takes place preferentially into excited states [1]. Furthermore the population of these excited states is selective: at most two values of n are significant. However the l and m distributions have not been established convincingly. With the exception of the work of Green et al. [2], most theories have neglected the coupling between substates of a given n, which are degenerate in hydrogenic systems [3, 4]. The case of the classical calculations [5] raises a different question: the ability of a classical calculation to reproduce correctly l and m distributions.

It has been shown by Burgdörfer [6] that the mixing between substates can be very important particularly due to the Stark effect caused by the residual target ion. Our aim is to study this problem in more details. We consider first the case of one-electron systems. The extention to many-electron systems will be the subject of a forthcoming contribution. It should be noted that the reactions studied here are very well suited to a study of the Stark mixing of sublevels. As shown before [9], two states are populated by a transition at a well defined distance (that of a pseudo crossing). Hence the Stark mixing can be isolated as the subsequent mixing between the various levels degenerate at infinity.

Our work is closely related to that of Green et al. [2] which we shall use as a standard to check the consistency of our model, though our effort is directed toward understanding the l and m distributions.

Our work is restricted to the energy region where the molecular theory of atomic collisions is valid (collision energy < 15 keV/amu). This is also the energy regime of interest for the fusion research.

In the first section of this paper we set up the frame of our calculations and discuss the technical problems related to a proper treatment of the process at large internuclear distances. In the second section we analyse the l and m distributions and propose a model which explains the main features of our results.

Atomic units are used unless otherwise stated.

(*) Equipe de recherche CNRS No 260.
2. Theoretical methods.

2.1 General considerations. — We have considered here the three reactions:

\[ \text{C}^6^+ + \text{H}(1s) \rightarrow \text{C}^5^+(n = 4) + \text{H}^+ \]  

(1a)

\[ \text{O}^8^+ + \text{H}(1s) \rightarrow \text{O}^7^+(n = 5) + \text{H}^+ \]  

(1b)

\[ \text{Ne}^{10^+} + \text{H}(1s) \rightarrow \text{Ne}^9^+(n = 6) + \text{H}^+ \]  

(1c)

Coupled state molecular calculations have been carried out for some of these systems by a number of authors (see references in [2]). We use the straight-line impact parameter approximation, i.e. the solution \( \Psi(t, R) \) of the time dependent Schrödinger equation is expanded in terms of molecular wave functions \( \chi(t, R) \):

\[ \Psi(t, R) = \sum_n a_n(t) \chi_n(t, R) \exp \left\{ -i \int^n \! \! dt' e_n(t') \right\} \]  

(2)

where:

- \( e_n \) is the molecular eigenenergy
- \( A \) is the projectile and \( B \) the target
- the internuclear distance \( R = BA \) is given by \( R = p + vt \) where \( p \) is the impact parameter and \( v \) the constant velocity. The angle \( \theta \) between the direction of \( v \) and \( R \) goes from \( -\infty \) to \( +\infty \). All these conventions are, for convenience, those of [7]. For the calculation of radial and rotational matrix elements [8] we have placed the origin of the electronic coordinate system on the ion. This choice is justified by the fact that we are interested in the substate distribution and only with this origin do the molecular states tend to the correct asymptotic limit. Correlatively we introduce an error on the description of the global charge transfer cross-section which occurs in the vicinity of a curve crossing (see discussion below). However the subsequent intrashell mixing will be correctly described. The results of Green et al. [2] support this assumption (see Fig. 2 of [2]: the « translation parameter » is close to 0.5 for all states on carbon for \( R > 9 \) a.u., which is equivalent to our choice of origin).

2.2 Description of systems. — The states retained in the expansion (2) for each system are:

\[ \text{C}^6^+ - \text{H} : \]

\( (5g\sigma)' + \) all states leading to \( \text{H}^+ + \text{C}^5^+(n = 4) \) — 11 states

\[ \text{O}^8^+ - \text{H} : \]

\( (6h\sigma)' + \) all states leading to \( \text{H}^+ + \text{O}^7^+(n = 5) \) — 16 states

\[ \text{Ne}^{10^+} - \text{H} : \]

\( (7i\sigma)' + \) all states leading to \( \text{H}^+ + \text{Ne}^9^+(n = 6) \) — 22 states

It should be noted that not all states degenerated at infinity need to be included in the calculation: the symmetry by reflection through the collision plane is conserved in the impact parameter method. The primed states are constructed as in our previous work [9] by smoothly interpolating diabatically the initial state at large distances (e.g. in the case of \( \text{Ne}^{10^+} - \text{H} \) the \( (7i\sigma)' \) state is identical to the \( 7i\sigma \) adiabatic state for internuclear distances smaller than 15 a.u. and is correlated to the entrance channel \( \text{H}(1s) + \text{Ne}^{10^+} \) for \( R \rightarrow \infty \)). In each case there is one pseudo-crossing which gives a dominant contribution to the charge exchange process in the energy range considered here: \( R_c \approx 8.0 \) a.u. for \( \text{C}^6^+ - \text{H}, R_c \approx 8.8 \) a.u. for \( \text{O}^8^+ - \text{H}, R_c \approx 9.8 \) for \( \text{Ne}^{10^+} - \text{H} \). In other terms we keep in the expansion (2) all states correlated with the substates of the most probable \( n \) value.

We give in figure 1 the potential curves of \( \text{Ne}^{10^+} - \text{H} \). Those of the other systems can be found elsewhere [2, 9].

2.3 Determination of amplitudes for different substates. — The OEDM (One Electron Diatomic Molecules) states lead at large internuclear distances to « Stark » hydrogenic states. For that reason, the present situation is an ideal one for the study of Stark mixing since the electric field is diagonal in our basis, that is contributes as a phase factor to the evolution of the basis states. To calculate the effect of Stark mixing on the population of levels of given \( l \) and \( m \), we have to make the transformation from « Stark » to « spherical » hydrogenic states. This transformation has been derived by many authors [10-13]. However their expressions are incorrect or undefined, with the exception of that of [13]. We discuss this problem further in appendix I. This transformation can be defined only if the phase convention of « Stark » to « spherical » hydrogenic states. This transformation has been derived by many authors [10-13]. However their expressions are incorrect or undefined, with the exception of that of [13]. We discuss this problem further in appendix I. This transformation can be defined only if the phase convention of « Stark » to « spherical » is well defined. Therefore we have to make explicit the phase convention of OEDM states in actual calculations. Finally, it should be noted that the OEDM use the internuclear axis as quantification axis, whereas we are interested in determining cross-sections with respect to a fixed axis. The transformation avoids spurious impact parameter dependencies. We discuss in detail these three points.

2.3.1 Sign of OEDM wave functions. — We use for the « Stark » hydrogenic states the phase convention of [15]:

\[ \Phi_{n_1,n_2}(\xi, \eta, \phi) = N_{n_1,n_2} e^{-i(l+1)(\eta/\sqrt{2})^m (\xi/\sqrt{2})^{m/2}} L_{n_1}^m(\xi/n) L_{n_2}^m(\eta/n) \Omega(\phi) \]  

(3)

where \( \xi, \eta, \phi \) are the parabolic coordinates: \( \xi = r + z; \eta = r - z; \phi \) and the Laguerre polynomials \( L_n^m \) are
defined as in expression (22.5.54) of [14]. The OEDM wave functions are determined by the method of [8]:

\[ \chi_\lambda(r, R) = A(\lambda) \cdot \Lambda(\mu) \cdot \Omega(\phi) \]  

(4a)

\[ A(\lambda) = (\lambda^2 - 1)^{m/2} (\lambda + 1)^{p} \exp(-\rho \lambda) \sum_{\ell=0}^{\ell_{\max}} g_{\ell}(R) \left[ (\lambda - 1)/(\lambda + 1) \right]^{\ell} \]  

(4b)

\[ M(\mu) = \sum_{s=0}^{s_{\max}} f_{s}(R) \cdot P_{\lambda+1}^{s}(\mu) \]  

(4c)

and \( \lambda, \mu, \phi \) are the prolate spheroidal coordinates:

\[ \lambda = (r_B + r_A)/R, \quad \mu = (r_B - r_A)/R, \quad \phi. \]

To relate the phase of (3) and that of \( \lim_{R \to \infty} \chi_\lambda(r, R) \), we only need to look at the form of these functions for \( r \to 0 \) and \( R \to \infty \). It is easy to see that \( \lim_{r \to 0} \phi_{nn,m}/\Omega(\phi) = N_{n_1,n_2,m} \) which is positive. The same limit corresponds to \( \lambda \to 1 \) and \( \mu \to 1 \) if the state is on atom B, or \( \mu = -1 \) if the state is on atom A (\( r_B \to r \) or \( r_A \to r \) respectively with \( R \gg r \)). From (4b):

\[ \lim_{\lambda \to 1} A(\lambda) = (\lambda^2 - 1)^{m/2} 2^p \exp(-\rho) g_0 \]  

which is positive since in [8] \( g_0 \) is always positive. It can be shown that:

\[ \lim_{\mu \to 1} M(\mu) = (1 - \mu^2)^{m/2} (2m - 1) \left[ \sum_s f_s(2m + s) / [s! (2m)!] \right] \]  

(6a)

\[ \lim_{\mu \to -1} M(\mu) = (1 - \mu^2)^{m/2} (2m - 1) \left[ \sum_s (-1)^s f_s(2m + s) / [s! (2m)!] \right] \]  

(6b)

which allows a determination of the sign of \( M(\mu) \) for \( r \to 0 \).

2.3.2 Transformation to spherical coordinates. — Once we have determined the transition amplitudes \( A_{nn,m} = a_{nn,m}(\infty) \) [7], we may calculate the amplitudes in the spherical basis as:

\[ A_{nm} = \sum_{n_1} \langle n_1 m | n_1 | m \rangle A_{nn_1,m}. \]  

(7)

The transformation is given in appendix I.

2.3.3 Stark effect at large distances. — The Stark effect appears in the basis through the behaviour of the molecular energies at large distances:

\[ \varepsilon_{nn,m}(R) \sim \varepsilon_{n}(\infty) + Z_B(Z - 1)/R + \frac{\alpha(n, n_1, m)}{R^2} + 0 \left( \frac{1}{R^2} \right). \]  

(8)

The first two terms can be neglected: they give a phase which is the same for all substates of given \( n \). The term in \( \alpha/R^2 \) comes from the linear Stark effect. As it depends on \( n_1 \) and \( m \), it influences \( A_{nm} \) through the transformation (7). In the calculation of \( \varepsilon \) for large \( R (R > 25) \) we keep all terms to sixth order in \( 1/R \). It is interesting to note that if we would use the spherical basis for our calculations at large distances, then the Stark effect would appear as a coupling term decreasing as \( 1/R^2 \) with internuclear distance.

2.3.4 Determination of the amplitude for a fixed axis of quantification. — We integrate the coupled equations [7] up to a maximum distance \( Z_M = \nu L \). Unless \( Z_M \) is much larger than the impact parameter \( \rho \), the internuclear axis will not lie along a fixed direction at the end of the integration as \( \rho \) is varied. This might introduce an error in the determination of \( A_{nm} \). A first solution would be to integrate until the condition \( Z_M \gg \rho \) is reached [2]. However this is not necessary. For \( Z > Z_M \), the rotational coupling in our rotating basis only expresses the fact that the states do not follow the rotation of the internuclear axis. Therefore we may obtain the same result by rotating the amplitudes determined at \( Z = Z_M \) onto a fixed direction. If we call \( A^{\alpha} \) the amplitudes determined in the rotating frame and if we call \( A^{\alpha^s} \) the amplitudes with the quantification axis along \( \theta \), then:

\[ a_{nm}^{\alpha^s} = \sum_m a_{nm}^{\alpha} \cdot R_{m,n}^{1}(\beta). \]  

(9)

The sign of \( \beta \) has to be defined in accordance with the convention used for the solution of the collision equations [7].
The matrix $R_{m'm}^{l}$ is not just the usual rotation matrix since we use basis states having a definite symmetry by reflexion through the collision plane:

$$R_{m'm}^{l}(\beta) = r_{m'm}^{l} \pm (-)^{m} r_{m'-m}^{l} \quad m' \neq 0, m \neq 0$$

(10)

$$R_{0m}^{l} = \sqrt{2} r_{m0}^{l} \quad R_{00}^{l} = r_{00}^{l}$$

where $r_{m'm}^{l}$ is as defined by Messiah [16].

We can verify that the transformations 2.3.1-4 are done consistently by checking that $A_{nm}^{l}$ does not depend on $Z_{M}$ and depends only loosely on $\rho$.

2.3.5 Extrapolation to infinity. — It is very important to note that the transformations 2.3.1 to 2.3.4 are essential for a correct determination of the transition amplitude unless ones integrates the coupled equations up to very large values of $Z$, as was done in [2]. In the present work we have stopped the integration for $Z_{M} \approx 15-20$ u.a., whereas in [2] $Z_{M} > 200$ u.a. Any error in one of the transformations 2.3.1 to 2.3.4 appears immediately through a spurious dependence of the results on $Z_{M}$. Hence we have a very strong test on the consistency of the various transformations.

The extrapolation for $Z > Z_{M}$ is carried out as follows. We first extrapolate the amplitudes, keeping the internuclear axis fixed, using the diagonal phase transformation 2.3.3. Then we transform these amplitudes into amplitudes for spherical states using 2.3.2 and finally make the rotation 2.3.3. This procedure, which is not correct for arbitrary times, is accurate for large enough $Z_{M}$. An extensive justification is given in appendix II.

The coupling between states such that in the separated atom limit $\Delta n = 0, \Delta t = \pm 1, \Delta m = 0$ is decreasing as $1/R^{2}$. The energy difference between these states is also decreasing as $1/R^{2}$. It can be checked that the transition probability between such states decreases rapidly enough as $t \to \infty$. This phenomenon should not be confused with the slowly decreasing rotational coupling ($\sim 1/R^{2}$) mentioned in 2.4. All other coupling terms decrease faster than $1/R^{2}$.

3. Results.

3.1 Reaction Mechanism. — We may check that our hypothesis on the reaction mechanism is correct by integrating the coupled equations from $t = 0$ to infinity, the initial state being the $(5g_{\alpha})$, $(6h_{\alpha})$ or $(7i_{\alpha})$ state depending on the system. The total transition probability as a function of impact parameter is plotted on figure 2. It varies very slowly with $\rho$ for $\rho \ll R_{c}$ and goes rapidly to zero for $\rho \gg R_{c}$ which confirms that transitions occur at the vicinity of the pseudo-crossing. We give in tables I-III the results of two different calculations:

(i) coupling between all states of the basis are kept;
(ii) only two states are coupled to the entrance channel : 4f_{\sigma} and 4f_{\pi} for C^{6+} - H, 5g_{\sigma} - 5g_{\pi} for O^{8+} - H and 6h_{\sigma} - 6h_{\pi} for Ne^{10+} - H.

Both sets of results are quasi identical which confirms the assumption of [9]: transitions at the vicinity of the crossing populate the $4f_{\sigma} - 4f_{\pi}$, $5g_{\sigma} - 5g_{\pi}$ or $6h_{\sigma} - 6h_{\pi}$ states. Subsequent coupling for $R > R_{c}$ distributes the population among the substates degenerate at infinity — hence extensive calculations are not required if only the total capture cross section is required.

3.2 Total Cross Sections for Given $l$. — The total cross sections for given $n$ and $l$ are listed in tables I-III. The distribution is very similar for the three cases considered here: it increases from $l = 0$ to $l = 2$. For $l > 2$ it has a plateau or decreases slightly, depending on the energy. This distribution is never a statistical one, which is at variance with calculations that do not include properly the intrashell mixing.

Fig. 1. — Purely electronic energies $E$ (in atomic units) of (NeH)^{10+} as a function of internuclear distance $R$ (in atomic units). For clarity, only $\alpha$ curves showing a pseudo-crossing between 5 and 20 a.u. have been plotted.

Fig. 2. — Total capture probability as a function of impact parameter (in atomic units) for a half collision. A: C^{6+} - H(1s) - shifted by $-0.1$, B: O^{8+} - H(1s), C: Ne^{10+} - H(1s) - shifted by $+0.1$. Arrows indicate the position of the pseudo-crossings.
Table I. — Electron capture cross sections for $\text{C}^6^+ + \text{H}(1s) \rightarrow \text{C}^6^+(n=4) + \text{H}^+$ in units of $10^{-16}$ cm$^2$.

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<th>Velocity (a.u.)</th>
<th>Total capture</th>
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(i) Eleven state calculation.
(ii) Only the $4s\pi$ and $4p\pi$ states are coupled to the initial state.
(iii) «Complete $l$-mixing» model.

Table II. — Electron capture cross section for $\text{O}^8^+ - \text{H}(1s) \rightarrow \text{O}^8^+(n=5) + \text{H}^+$ in unit of $10^{-16}$ cm$^2$.

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(i) Full 16 state calculation.
(ii) Only the $5g\sigma$ and $5g\pi$ states are coupled to the initial state.
(iii) «Complete $l$-mixing» model.
Table III. — Electron capture cross section for Ne$^{10+}$ – H(ls) → Ne$^9+$(n = 6) + H$^+$ in units of 10$^{-16}$ cm$^2$.

a) $l$ distribution.

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<td>3.9</td>
<td>8.1</td>
<td>10.8</td>
<td>12.3</td>
<td>13.1</td>
<td>13.4</td>
</tr>
<tr>
<td>ii</td>
<td>54.1</td>
<td>3.5</td>
<td>9.4</td>
<td>11.8</td>
<td>11.4</td>
<td>9.6</td>
<td>7.7</td>
</tr>
<tr>
<td>iii</td>
<td>3.4</td>
<td>6.8</td>
<td>9.2</td>
<td>10.6</td>
<td>11.4</td>
<td>11.8</td>
<td></td>
</tr>
</tbody>
</table>

(i) Full 22 state calculation.
(ii) Only the 6h a and 6 h n states are coupled to the initial state.
(iii) « Complete l mixing » model.

Our $l$ distribution is very similar to that of Green for low velocities. However it differs appreciably from his results for the highest velocities considered here. There are still some differences with the work of [2]. In [2] translation factors have been used, which is not the case in our work. However, as we have mentionned in 2.1, in the region of interest for the $l$, $m$ distributions the parameters of his translation factors make his calculations equivalent to ours with the origin on the projectile. We do calculations only for the main process (populating one state) whereas, in [2] the various channels are fully coupled. However, as recognized in [2], the population of the various $n$ states can be calculated independently. Hence there is no obvious reason to the discrepancy between the results of [2] and ours at high energies.

It is worth noting that the rotation of the parabolic states is rather difficult to describe. Rotation couples states with the same $l$ and different $m$ values and each parabolic state is a linear combination of spherical states. Hence the independence of our results on the end point of the integration is a very strong test on the validity of our calculations (integration of coupled equations, transformation from parabolic to spherical basis, transformation to a fixed reference axis).

We give in tables I-III the $m$ distribution, the axis of quantification being the initial direction of the velocity of the projectile. The $m = 0$ and $m = 1$ states are nearly equally populated, whereas the population of various $m$ values decreases as $m$ increases for $m \geq 2$. The $m$ distribution allows us to understand the gross feature of the $l$ distribution. Assuming a statistical distribution among possible $l$ values for a given $m$, we obtain the results (iii) of tables I-III, referred to as « complete l mixing » model. The general picture of the $l$ distribution is very well reproduced by this model, especially at low energies. This can be easily interpreted as a consequence of the mixing of $l$ states through the linear Stark effect.

Hence the $m$ distribution is more significant than the $l$ distribution. We should note however some deviations, most noticeably at the highest energies.
3.3 Interpretation of the $m$ distribution. — In order to interpret the $m$ distribution, one needs information on two possible sources of asymmetry:

(i) asymmetry in the primary process (around the curve crossing) which explains the charge exchange;

(ii) rotation of the electronic states after their population at the curve crossing. As we have mentioned earlier, in our rotating basis, the rotational coupling also takes care of the inability of the atomic states to follow the rotation of the internuclear axis at large internuclear distances.

In order to get information on the primary process, we have made again calculations on a half collision, starting from the distance of minimum approach. However we stopped the integration for a value of $Z$ such that the internuclear distance is a little larger than $R_c$ ($R_{\text{max}} = 8.5$ for $\text{C}^6+; R_{\text{max}} = 10$ for $\text{O}^8+$ and $\text{Ne}^{10+}$). We analyse the $m$ distribution, using the direction of the incident velocity as quantization axis. This is done by rotating the molecular states as described in 2.3.4, which implicitly supposes that the states of the system can be approximated by a superposition of atomic states for $R = R_{\text{max}}$. Results are given in table IV. We obtain the striking result that the state populated by charge exchange at the vicinity of the pseudo-crossing has a dominant projection $m = 0$ with respect to the direction of the initial relative velocity of the nuclei. The selectivity of this process increases with energy. Only for the lowest velocities is there an evidence that the $m$ distribution changes with increasing impact parameter as could be expected if the direction of the internuclear axis would be determinant.

It is not trivial, however, to relate the data of table IV to the actual distribution of $m$ values observed in a full collision. In the collision, the system goes twice through $R_c$ and the final $m$ distribution will depend in a complicated way on the rotation of the internuclear axis between the two passages through the pseudo-crossing.

4. Conclusion.

We have shown that, in one electron systems, the $l$ distribution of atomic states formed by charge exchange is not representative of the charge exchange process itself: Stark mixing is strong enough to mix the various $l$ substates. In fact, geometrical effects related to the $m$ distribution are dominant. It is the $m$ distribution which creates the main constraint on the $l$ distribution. This observation justifies the effort that should be made to measure the polarisation of the radiation emitted by decay of the excited states.

It is not obvious that this conclusion can be extended in a straightforward way to the case where the incoming ion carries a core. In the latter case, the core inhibits the linear Stark effect which may have consequences both on the overall charge exchange cross section and on the $l$ and $m$ distributions. Still the present work can be used as a basis for comparison with more complex cases.

Acknowledgments.

The author acknowledges the useful contributions and stimulations from his colleagues of the Laboratoire des Collisions Atomiques. The material of the appendix is based on a collaboration with J. Hanssen and Dž. Belkić. Thanks are due to T. Grozdanov for useful discussions and suggestions and for communication of results in advance of publication.

Table IV. — Distribution of probabilities over $m$ values for a half collision. Integration has been stopped for $R = 8.5$ a.u. ($\text{C}^6+ - \text{H}$) or $R = 10.0$ a.u. ($\text{O}^8+ - \text{H}$ and $\text{Ne}^{10+} - \text{H}$).

<table>
<thead>
<tr>
<th>Velocity (a.u.)</th>
<th>Impact parameter (a.u.)</th>
<th>0.2</th>
<th>0.5</th>
<th>0.8</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\text{C}^6+ - \text{H}$</td>
<td>$m = 0$</td>
<td>0.23</td>
<td>0.28</td>
<td>0.31</td>
</tr>
<tr>
<td></td>
<td>$m = 1$</td>
<td>0.002</td>
<td>0.007</td>
<td>0.007</td>
</tr>
<tr>
<td></td>
<td>$m = 2$</td>
<td>0.001</td>
<td>0.001</td>
<td>0.001</td>
</tr>
<tr>
<td>$\text{O}^8+ - \text{H}$</td>
<td>$m = 0$</td>
<td>0.32</td>
<td>0.37</td>
<td>0.49</td>
</tr>
<tr>
<td></td>
<td>$m = 1$</td>
<td>0.001</td>
<td>0.006</td>
<td>0.001</td>
</tr>
<tr>
<td></td>
<td>$m = 2$</td>
<td>0.001</td>
<td>0.001</td>
<td>0.001</td>
</tr>
<tr>
<td>$\text{Ne}^{10+} - \text{H}$</td>
<td>$m = 0$</td>
<td>0.17</td>
<td>0.23</td>
<td>0.23</td>
</tr>
<tr>
<td></td>
<td>$m = 1$</td>
<td>0.001</td>
<td>0.005</td>
<td>0.009</td>
</tr>
<tr>
<td></td>
<td>$m = 2$</td>
<td>0.003</td>
<td>0.003</td>
<td>0.001</td>
</tr>
</tbody>
</table>

The probabilities for $m > 3$ are not given because they all have small values ($\sim 10^{-3}$ or less). $\varepsilon$ means that the probability is $< 10^{-3}$.
Appendix L — Transformation from parabolic to spherical hydrogenic states.

The transformation matrix from the parabolic states $\Phi_{nnlm}(\xi, \eta, \phi)$ to the spherical states $\psi_{nlm}(r, \theta, \phi)$ has been worked out by Park [10] and Hughes [11]. However, these authors fail to state explicitly the phase convention in the definition of the basis states. This point has already been discussed by Belkic [13].

Another method consists in noting first that the parabolic states diagonalize the matrix elements of $Z$. Hence one may obtain the transformation matrix by diagonalizing the matrix elements $Z_{n,l-1,m}^{n+1,m}$ of $Z$ in the spherical basis [12]. We then have to find some method to determine the phase of the states constructed by diagonalization so that it agrees with the definition of $\Phi_{nnlm}$. We use the following definition for the hydrogenic states [15].

1) $\Phi_{nnlm}$ is defined in (3) with

$$\Omega(\phi) = \frac{e^{i\mu\phi}}{\sqrt{2\pi}}, \quad N_{nnlm} = \frac{\sqrt{2}}{n_l^{2+|m|}} \left( \frac{n_1! n_2!}{(n_1 + |m|)! (n_2 + |m|)!} \right)^{1/2}$$  \hspace{1cm} (A.1)

2) $\Psi_{nlm} = R_{nl} Y_{nlm}(\theta, \phi)$.

We use for $Y_{nlm}(\theta, \phi)$ the definition of Messiah [16] (expression (93) of appendix IB) and

$$R_{nl} = N_{nl}^{-1/2} e^{-l/2} L_{n-l}^{l+1}(x), \quad x = \frac{2r}{n}$$  \hspace{1cm} (A.3)

with $N_{nl} = \frac{2}{n^2} \left( \frac{n-l!}{(n+l)!} \right)^{1/2}$.

If one writes :

$$\Psi_{nlm} = \sum_{n_1=0}^{n-|m|-1} \langle nn_1 m/nlm \rangle \Phi_{nn_1,m}$$  \hspace{1cm} (A.4)

then Belkic has shown that :

$$\langle n_1 m | nlm \rangle = (-1)^{\eta+l+(|m|-m)/2} (2l+1)^{1/2} \left( \frac{\xi (n-1)}{3}, \frac{\eta (n-1)}{3}, \frac{l}{2} \right)$$  \hspace{1cm} (A.5)

The consistency of this formula with the definitions can be easily verified by explicit calculations. The diagonalization method starts by calculating :

$$Z_{nlm}^{n+1,m} = Z_{nlm}^{n+1,m} = - \left[ \frac{(l+1)^2 - m^2}{(2l+1)(2l+3)} \right]^{1/2} \frac{3}{2n^2} \left[ (n^2 - (l+1)^2)^{1/2} \right].$$  \hspace{1cm} (A.6)

Note the error of sign in expression (63.5) of [17]. The correspondence between the states that diagonalize $Z$ and the parabolic states can be easily achieved by noting that in the parabolic basis $\langle Z \rangle = \frac{1}{2} n(n_1 - n_2)$.

The phase can be fixed by looking at the form of the functions for $r \to 0$. We write

$$\Phi_{nnlm} = \sum_{r=0}^{r_{|m|}} a_r \psi_{nlm} \sim a_{|m|} \psi_{nlm}$$  \hspace{1cm} (A.7)

Noting that $\eta = r(1 - \cos \theta)$, $\xi = r(1 + \cos \theta)$ and using the small $r$ expansion of both $\psi_{nlm}$ and $\Phi_{nnlm}$, we get ($\mu = |m|$)

$$a_{\mu} = (-)^{\mu} \frac{(2\mu + 1)!}{\mu! \sqrt{2\mu + 1}} \left( \frac{n_1! n_2! (n_2 + \mu)!}{n_1! n_2!} \right)^{1/2} \left( \frac{(n - \mu - 1)!}{(n + \mu)! (2\mu)!} \right)^{1/2}$$  \hspace{1cm} (A.8)

which fixes the phase of the parabolic states. It can be checked easily that the results are identical to those given by (A.5) and are at variance with the explicit ones given by [12].
Appendix II. — Discussion of the procedure to extrapolate the solutions for \( Z_M > Z \).

For large internuclear distances we have taken account of the fact that the states do not follow the rotation of the internuclear axis. Also we neglect the variation in orientation of the force between the residual charge and the final atomic state. We discuss here the validity of these two conditions.

1) Rotation.

If for \( R > R_M \), the rotational coupling matrix elements can be replaced by their asymptotic value, then the electronic state does not rotate.

We write the coupled equations of our model for large internuclear distances, i.e. neglecting radial couplings (however this is only for simplicity and it does not modify our argument)

\[
\dot{a}_{n_1m} = - \frac{i}{\nu} e(n_1, m) a_{n_1m} + \sum_{n_1m'} \dot{\theta} \langle \phi_{n_1m} | iL_y | \phi_{n_1m'} \rangle a_{n_1m'}.
\]  
(A.9)

In this expression, \( \phi_{n_1m} \) is the parabolic atomic state, \( L_y \) is the component of the angular momentum operator perpendicular to the collision plane and \( e(n_1, m) \) is the molecular eigenenergy. The matrix elements of \( iL_y \) are taken between asymptotic states since our hypothesis is that the matrix element of \( iL_y \) has reached its asymptotic value.

We write the transformation (A.4) with the notation:

\[
\phi_{n_1m} = \sum_l c^n(n_1, l) \phi_{lm}, \quad \phi_{lm} = \sum_{n_1} c^n(l, n_1) \phi_{n_1m}.
\]  
(A.10)

and introduce the amplitude of the spherical states:

\[
a_{lm} = \sum_{n_1} c^n(n_1, l) a_{n_1m}; \quad a_{n_1m} = \sum_l c^n(l, n_1) a_{lm}.
\]  
(A.11)

We get the coupled equation:

\[
\dot{a}_{nl} = - \frac{i}{\nu} \sum_{l'} \sum_{m} e(n_1, m) c^n(n_1, l) c^{n'}(l', n_1) a_{l'm} + \sum_{n_1} \dot{\theta} \langle \phi_{n_1m} | iL_y | \phi_{n_1m'} \rangle a_{n_1m'}.
\]  
(A.12)

where we have used the fact that \( L_y \) is diagonal in \( l \).

We now introduce states \( \Phi \) that are fixed in space:

\[
\Phi_{lm} = \sum_{n_1} r^{n_1m}(\theta) \phi_{lm}; \quad \phi_{lm} = \sum_{n_1} r^{n_1m}(-\theta) \Phi_{lm}.
\]  
(A.13)

with the corresponding amplitudes:

\[
\Lambda_{lm} = \sum_m a_{lm} r^{n_1m}(-\theta).
\]  
(A.14)

Starting from:

\[
\dot{\Lambda}_{lm} = \sum_{m'} a_{lm'} \left\{ \frac{d}{dt} r^{n_1m}(-\theta) \right\} + \sum_{m'} r^{n_1m}(-\theta) \dot{a}_{lm'}.
\]  
(A.15)

it can readily be shown that:

\[
\frac{d}{dt} r^{n_1m}(\theta) = \dot{\theta} \sum_{n_1} \langle \phi_{lm'} | iL_y | \phi_{lm} \rangle r^{n_1m}(\theta)
\]  
(A.16)

so that our final coupled equations for \( \Lambda \) are:

\[
\dot{\Lambda}_{lm} = - \frac{i}{\nu} \sum_{n_1} \sum_{l'} \sum_{m'} e(n_1, m) c^n(n_1, l) c^{n'}(l', n_1) r^{n_1m'}(-\theta) r^{n_1m'}(\theta) \Lambda_{l'm'}.
\]  
(A.17)

This equation does not include \( \dot{\theta} \) which proves our point.

2) Orientation of the « Stark» effect.

Still our equation (A.17) depends on \( \theta \). This is because the direction of the force is along the internuclear axis. We may illustrate this fact by noting that, in an expansion over \( 1/R \), the first order term is \( r \cdot R/R^3 \), where \( r \) is the electronic coordinate.
This term has an axial and transverse component. Expression (A.17) includes this orientation effect in a completely general form. Our extrapolation procedure for \( Z > Z_m \) is equivalent to keeping only the longitudinal term. We will show now under what condition the transverse term can be neglected. Let us call \( \theta_m \) the angle that the internuclear axis makes with its final direction when \( Z = Z_m \). We rewrite (A.17) as:

\[
\hat{A}_{lm} = -\frac{i}{v} \sum_{n_1} \sum_{l'} \sum_{m'} \sum_{m} \varepsilon(n_1, m) c^{m}(n_1, l) c^{m'}(l', n_1) A_{l'm'} \times \sum_{\mu} \sum_{\mu'} r_{\mu}^{m'}(-\theta_m) r_{\mu'}^{m}(\theta_m) r_{\mu}^{m}(\theta - \theta_m).
\] (A.18)

In our procedure, we take into account only the diagonal molecular terms for \( Z > Z_m \), the axis being kept fixed in the direction \( \theta_m \). This means that we use the approximate equations:

\[
\dot{b}_{n,m} = -\frac{i}{v} \varepsilon_{n,m} b_{n,m}.
\] (A.19)

Following steps similar to (A.9)-(A.17), we obtain the amplitude for the spherical states referred to a fixed direction as:

\[
\dot{B}_{l,m} = -\frac{i}{v} \sum_{n_1} \sum_{l'} \sum_{m'} \sum_{m} \varepsilon(n_1, m) c^{m}(n_1, l) c^{m'}(l', n_1) r_{l}^{m'}(-\theta_m) r_{l}^{m}(\theta - \theta_m) B_{l'm'}.
\] (A.20)

The latter equation is equivalent to (A.18) only if \( |\theta - \theta_m| \ll 1 \). As \( |\theta| < |\theta_m| \) this will be certainly the case if \( \theta_m \ll 1 \), which confirms that the transverse term goes to zero faster than the longitudinal term. However the convergence is even stronger with the procedure we use since our condition is not \( \theta_m \ll 1 \) but \( |\theta - \theta_m| \ll 1 \) and, for each \( \theta \), every contribution is weighted by \( \varepsilon(n_1, m) \) which goes to zero at least as \( 1/R^2 \). This explains why our results are insensitive to \( Z_m \) even for rather small values of \( Z_m \).

In their model Grozdanov and Belić [18] also neglect the rotation. However they do take into account the orientation effect since this can be done exactly if the interaction potential between the proton and the final atom is supposed proportional to \( r/R^3 \).

**References**