

# LOW-ENERGY ROTATIONAL EXCITATION OF H<sub>2</sub> AND N<sub>2</sub> BY POSITRON IMPACT. II – COMPARISON WITH ELECTRON IMPACT

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## ABSTRACT

Low-energy collisional excitation of rotations in H<sub>2</sub> and N<sub>2</sub> by impact with slow positrons in the gas phase is considered by carrying out a Space-Frame (SF) dynamical calculation at energies well below the positronium formation threshold, is compared with similar calculations with electron projectiles.

## RESUMEN

Se consideran excitaciones por colisiones de baja energía de rotaciones en H<sub>2</sub> y en N<sub>2</sub> por impacto con positrones lentos en la fase gaseosa llevándose a cabo un cálculo dinámico en el sistema de referencia espacial a energías bien por debajo del umbral de formación del positronium y se compara con cálculos similares con proyectiles electrónicos.

## I. INTRODUCTION

The experimental and computational study of low-energy positron scattering from molecular gases, both diatomic species and polyatomic targets, has a relatively long history which is chiefly related to the fundamental interest in the consequences of positron annihilation in gases and in the effects of slowing down positron beams in several media of applied relevance [1-3].

One of the complications created by the use of antiparticles in low-energy processes is the existence of additional channels which are not present in the case of electron beams. Thus, we know of the possibility of forming the positronium (Ps) compound, that adds a distinct 'reactive' channel to the theoretical description of the above processes [1], or that the particle-antiparticle decay channel, whereby the pick off by the positron of a bound electron leads to the emission of 2 or 3  $\gamma$  photons, can leave molecular cations within the gas and therefore strongly modify the collisional process. In the present study, we therefore compare the behaviour of this leptonic anti-particles with that of its counterpart, the electron particle at the same collision energies and for which none of the above channels exist.

## II. THE SPACE-FRAME DYNAMICS

In the present calculations we shall treat the N<sub>2</sub> and H<sub>2</sub> molecular targets as rigid rotors, disregarding from the time being the effects of vibrational excitations during the rotational energy transfer collisions. Furthermore, as reported in the following Section, the interaction with the molecules will be described by a local, energy-independent effective potential between the impinging particle and the rotating target and the electron-molecule interaction will further include a localized form of exchange interactions. The asymptotic target states are given in both cases by simple spherical rotors

$$H_{\text{rot}}(\hat{R}_{\text{eq}})Y_{j m j}(\hat{R}_{\text{eq}}) = \frac{\hbar^2}{2I} j(j+1)Y_{j m j}(\hat{R}_{\text{eq}}) \quad (1)$$

with  $I$  being the isolated molecule moment of inertia [4] and  $\hat{R}_{\text{eq}}$  the space orientation of the molecular bond, kept at its equilibrium value. Hence, the total scattering wavefunction is given as

$$\Psi_n(E, r_p, R_{\text{eq}}) = \sum_f u_{i \rightarrow f}(r_p, E) r_p^{-1} Y_f(\hat{R}_{\text{eq}}) \quad (2)$$

where  $|f\rangle$  denotes the  $|j_f m_f\rangle$  final states of the molecule involved in the expansion and the  $u_{i\rightarrow f}(r_p, E)$  are the channel components of the scattering wavefunction, to be determined by solving the usual Schrödinger equation subject to its scattering boundary conditions. All details of the present computations were given in the preceding paper (I) and therefore will not be repeated here.

The numerical convergence tests of the values of the K-matrix were carried out as in the preceding paper (I) and electron-molecule cross section were also considered to be converged within  $10^{-3}$  Å of their values.

### III. THE POSITRON-MOLECULE AND ELECTRON-MOLECULE INTERACTIONS

If one starts in the asymptotic region of the interaction, where charge overlap effects have vanished, one can immediately write the dipole leading term of the polarisation part of the full potential  $V_{pcp}$  [8]

$$V_{pcp}(r_p) \sim V_{pol}(r_p) = -\frac{1}{2r_p^4} \left\{ \alpha_0(R) + \alpha_2(R) P_2(\hat{R} \cdot \hat{r}_p) \right\} \quad (3)$$

where  $\alpha_0$  is the spherical dipole polarisability of the target molecule at its geometry  $R$ ,  $\alpha_2$  is its non-spherical term and the Legendre polynomial depends on the molecular frame angle  $\vartheta = \arccos(\hat{R} \cdot \hat{r}_p)$ . We have employed experimental values for such quantities [9]. The present  $V_{pcp}$  is based on the correlation energy of a localized  $e^+$  in an  $e^-$  gas, and its hybridization with the correct asymptotic form of equation (3). Earlier on [10,11] a similar approach was applied to the problem of a light impurity in an electron gas. In those methods, the electron gas is described by a set of interacting bosons representing the collective excitations in the random-phase-approximation. Further, Boronski and Nieminen [12] described the density-functional theory of the electron-positron system, and presented the results on the positron-electron correlation energy as a function of the density parameter  $r_s$  [10-12] for different  $n_+(r_s)/n_-(r_s)$  ratios including the case of one positron in a homogeneous electron gas. Here  $n_+$  and  $n_-$  denote the densities of positrons and electrons, respectively.

It therefore follows that the total  $V_{pcp}$  potential for the  $e^+$ -molecule system can now be assembled by writing

$$\begin{aligned} V_{pcp}(r_p | R) &= V_{corr}(r_p | R) \text{ for } r_p < r_c \\ &= V_{pol}(r_p | R) \text{ for } r_p > r_c \end{aligned} \quad (4)$$

The connecting parameter  $r_c$  is usually around 4.0  $a_0$  for the present system and varies depending on the chosen multipolar coefficient of the final expansion. The total  $e^+$ -molecule interaction potential can now be obtained in a local form and will also include the exact electrostatic interaction  $V_{st}(r_p)$

$$V_{tot}(r_p | R) = V_{st}(r_p | R) + V_{pcp}(r_p | R) \quad (5)$$

The corresponding analysis for electrons as projectiles has been already presented elsewhere and will not be discussed here. Suffices it to say that its final form will be similar as that of equation (5) but with the addition of exchange interaction:

$$V_{tot}(r_e | R) = V_{st}(r_e | R) + V_{ex}(r_e | R) + V_{ecp}(r_e | R) \quad (6)$$

The above interactions can be further expanded over the usual set of Legendre polynomials

$$V_{tot}(r_p | R) = \sum_{L=0}^{\infty} V_L(r | R) P_L(\hat{r} \cdot \hat{R}) \quad (7)$$

the coefficients only take even  $L$  values and provide the anisotropic coupling potential terms needed in the scattering eq.s where they are directly included in equation (7) of paper (1), both for  $e^-$  and  $e^+$  projectiles.

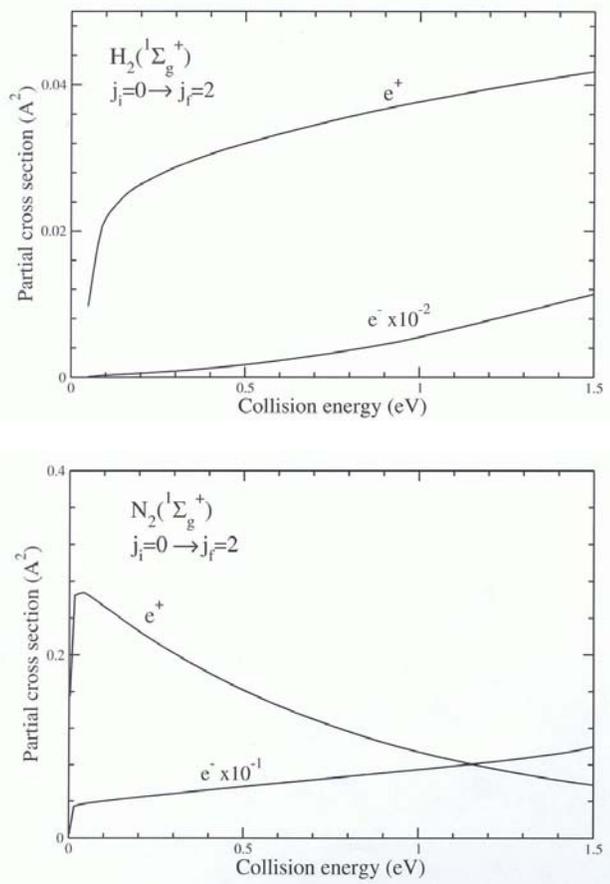
### IV. ELECTRON AND POSITRON IMPACT EXCITATION

Due to the dramatic increase in recent years on the breadth and variety of experimental and theoretical data which have been gathered on the low-energy behaviour of leptonic projects, like  $e^+$  and  $e^-$ , when undergoing collisions by injection into molecular gases [2,3], it is of some interest to look a bit more in detail at their comparative behaviour when taken to produce rotational heating of the molecules in the ambient gas. An extensive review of such data on diatomic and polyatomic targets has recently provided [14] a great deal of insight on the comparative behaviour of those projectiles.

The  $(0 \rightarrow 2)$  excitation cross sections are compared, over the same energy range, in the two panels of Figure 1: the electron scattering calculations are from ref. [13].

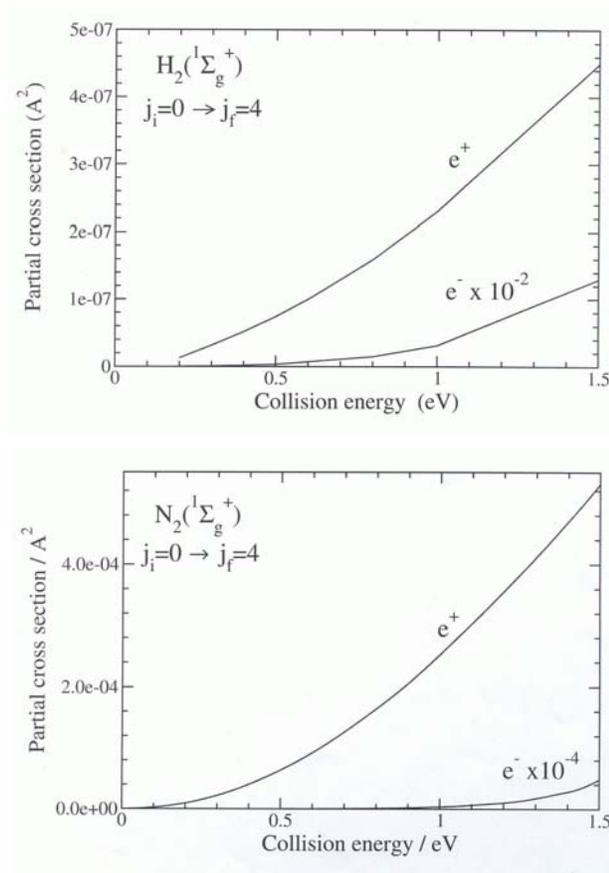
In the case of molecular hydrogen (upper panel) we see that the positron results are about two orders of magnitude smaller than in the case of the  $e^-$  excitation cross sections. The repulsive static interaction, in the case of the  $e^+$  lepton, keeps the projectile largely away from the inner interaction

regions and therefore causes a reduction of the range of action over which the coupling anisotropy can apply a rotational torque to the target molecule. Such an effect is also present in the case of  $N_2$  where, however, the reduced efficiency of the positron-impact excitation process is particularly evident over the region of the shape resonance. Around 2 eV of collision energy, in fact, the  $(0 \rightarrow 2)$  excitation cross sections for electron impact is about  $8.0 \text{ \AA}^2$ , to be compared with that from positron scattering of about  $0.025 \text{ \AA}^2$ .



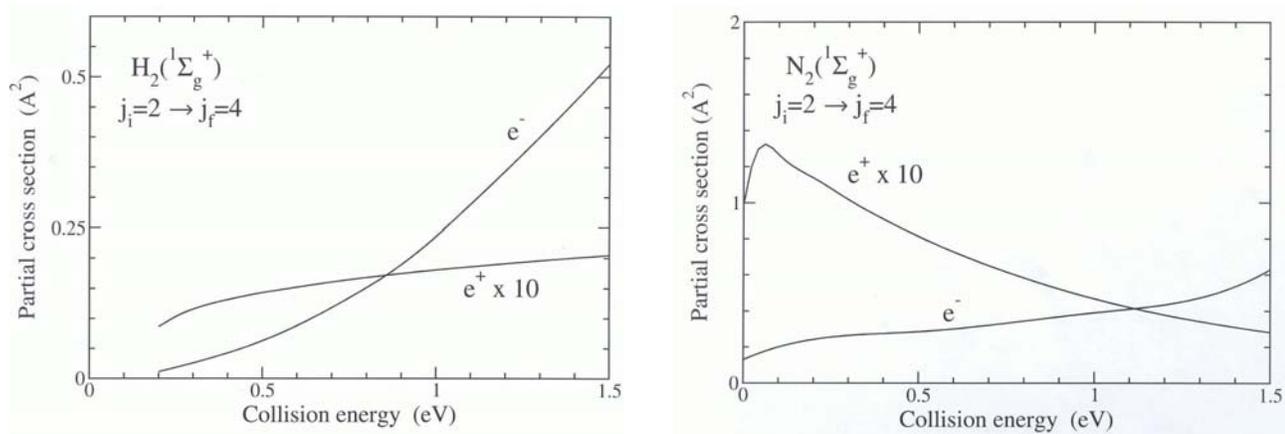
**Figure 1.** Comparison of computed partial integral cross sections for the  $(j_i = 0 \rightarrow j_f = 2)$  process induced by the two leptonic projectiles on  $H_2$  (upper panel) and  $N_2$  (lower panel) molecules. The computed values for  $e^-$  are from ref. [13]

The additional calculations of Figure 2 show the same comparison with regard to the  $(0 \rightarrow 4)$  excitation cross sections. In the case of the  $H_2$  target the comparison shows similar results to those obtained for the  $(0 \rightarrow 2)$  excitations of figure 1: the inelastic efficiency for the  $e^+$  lepton is about  $10^{-2}$  times lower than for electron impact. For the  $N_2$  molecule, on the other hand, the difference is even greater, especially in the resonance region where the electron impact excitation increases by more than one order of magnitude.



**Figure 2.** Same as figure 1 but for the state-to-state  $(j_i = 0 \rightarrow j_f = 4)$  rotational excitation processes. See caption of Figure 1 for details.

When starting the excitation process from a molecular state higher than  $j_i = 0$ , the two molecules are shown in Figure 3 to be excited by  $e^+$  and  $e^-$  from their  $j = 2$  initial level. In both cases we see that the existence of the electron-impact shape resonances (beyond 3 eV for  $H_2$  and around 2 eV for  $N_2$ ) play a significant role in enhancing rotationally inelastic probabilities, while nothing of the sort exists for the positron excitation processes. Furthermore, we see that both sets of cross sections are markedly larger than the same excitation jumps  $(\Delta_j = 2)$  from the  $j_i = 0$  levels shows by the Figure 3: the differences between the two leptonic excitation collision cross sections are about one order of magnitude and the cross sections themselves are more than a factor of ten larger than the  $(0 \rightarrow 2)$  cross sections of Figure 3. This suggests that initially 'hot' gaseous environments could induce more efficiently the further heating of the molecular gas, thereby more efficiently provide a cooling environment both for  $e^+$  and  $e^-$  beams. On the whole, however, these calculations indicate that between the two leptons it is again the electron that turns out to be more efficient in rotationally heating the  $H_2$  and  $N_2$  molecules and that  $N_2$  excitation probabilities are larger than those of  $H_2$  for both types of projectiles.



**Figure 3.** Comparison of impact excitation of H<sub>2</sub> (upper panel) and N<sub>2</sub> (lower panel) molecules from their excited rotational level  $j_i = 2$  into  $j_f = 4$  level by collisions with the  $e^+$  and  $e^-$ . All the results are from present calculations.

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