

Ro-vibrational close coupling study of positron–hydrogen molecule scattering using the parameter-free model correlation polarization potential

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Abstract

In this paper, we have presented the ro-vibrational laboratory frame close coupling (LFCC) calculation for the positron–hydrogen molecule scattering process. We have reported here (integrated) total cross section as well as vibrational and rotational excitation cross sections in the low-energy region of the incident positron. To calculate the scattering parameters we have used the positron correlation polarization potential (PCOP), which is especially meant for the positron as the incident particle. The present results are compared with the existing elaborate theories and the measured values. The present total cross sections agree well with the measured values, whereas the absolute values of the $0 \rightarrow 1$ vibrational excitation cross sections differ marginally. There are some differences between the present result and the other theoretical predictions. The reasons behind the differences are discussed.

Introduction

Atomic/molecular collision physics is an important area of research where the positron is employed as a probe. To the theoretician the positron–atom/molecule collision is very important in the sense that the sign of the static potential due to the repulsive interaction between the positron and the target is positive, whereas the lower-order term in the polarization potential is negative. So a good deal of cancellation in the potential occurs when one tries to compute the scattering parameters. Thus, the theoretically calculated scattering parameters using a model polarization potential when compared with the measured values give an estimate of the accuracy of the polarization potential used.

The positron (electron)–molecule scattering calculation is complicated due to the inclusion of the nuclear degrees of freedom in the scattering calculation, especially in the low-energy region where the projectile spends a longer time with the target molecule. To tackle this situation, the well-known Born–Oppenheimer (B–O) approximation is invoked in the calculation. Under the B–O approximation, the electronic and

nuclear coordinates of a molecule are treated as the fast and slow variables, respectively.

The molecular collision calculation is more complicated than the bound state calculation due to the introduction of the projectile coordinate. This problem has been tackled using different methods, which put restriction on the nuclear motion. These lead to different models employed in positron (electron)–molecule collision processes, namely, the body-frame-fixed nuclei (BFFN) model, the adiabatic nuclei (AN) model, the rotational laboratory frame close coupling (LFCC) approximation, the body-frame vibrational close-coupling (BFVCC) approximation (Armour 1988, Ghosh and Mukherjee 1996, Gianturco and Mukherjee 1997, 2001), etc. However, the applicability of the different coupling schemes depends on the energy of the incident particle.

Present work

Here we have presented a ro-vibrational LFCC calculation in a low-energy positron–hydrogen molecule collision including both the rotational and vibrational motion of the nuclei

dynamically. To the best of our knowledge, so far there are two calculations that have been performed to predict vibrational excitation cross sections for the above-mentioned process. One is the calculation of Gianturco and Mukherjee (1997, 2001) including only the vibration of the molecule dynamically, and the other is the calculation performed by Sur and Ghosh (1985) using the ro-vibrational coupling method. Sur and Ghosh used the polarization potential of Henry and Lane (1969) and a simplified version of the target electronic wavefunction, namely the Wang wavefunction. The Henry–Lane polarization potential does not include any specific positron signature. In the present calculation we have used a more acceptable model, the positron correlation polarization (PCOP) potential, meant for the positron as an incident particle and a more elaborate molecular wavefunction of the hydrogen molecule. Our main objective in the present work is to see the effect of dynamical coupling of the nuclear motions (rotations and vibrations) in the scattering process and predict theoretically more accurate and more *ab initio* total, vibrational and rotational excitation cross sections.

Theory

To describe the scattering of a positron by a rotating and vibrating molecule in its electronic ground state, one has to solve the familiar Schrödinger equation

$$(H - E)\Psi = 0 \quad (1)$$

subject to the usual scattering boundary conditions. Here, H and Ψ are the total Hamiltonian and the total wavefunction of the positron–molecule system. In the present ro-vibrational LFCC formalism under B–O approximation, the total Hamiltonian is given by

$$H \equiv H(\vec{r}_p) + H_{el}(\vec{r}_e) + H_{vib}(R) + H_{rot}(\hat{R}) + V_{p-mol}(\vec{r}_p, \vec{r}_e, \vec{R}), \quad (2)$$

where \vec{r}_p is the positron coordinate measured from the centre of mass of the system, \vec{r}_e collectively denotes the molecular electronic coordinates and \vec{R} is the inter-nuclear set of coordinates of the molecule. $H(\vec{r}_p)$ is the kinetic energy operator for the incident positron, $H_{vib}(R)$, $H_{rot}(\hat{R})$ and $H_{el}(\vec{r}_e)$ are the vibrational, rotational and electronic Hamiltonians of the target molecule, respectively. $V_{p-mol}(\vec{r}_p, \vec{r}_e, \vec{R})$ represents the positron–molecule interaction. The total wavefunction in the ro-vibrational LFCC model is given by

$$\Psi_{vj'l}^{JM}(\vec{r}_p, \vec{r}_e, \vec{R}) = \chi_0(\vec{r}_e, \vec{R}) \sum_{v'} \sum_{j'} \sum_{l'} r_p^{-1} u_{v'j'l'}^{Jvj'l}(r_p) \times \Upsilon_{j'l'}^{JM}(\hat{r}_p, \hat{R}) \phi_{v'}(R), \quad (3)$$

where $\chi_0(\vec{r}_e, \vec{R})$ is the ground-state electronic wavefunction that parametrically depends on \vec{R} . $\phi_{v'}(R)$ is the vibrational wavefunction of the molecule, v labels the vibrational quantum number. The angular basis function Υ is given by

$$\Upsilon_{j'l'}^{JM}(\hat{r}_p, \hat{R}) = \sum_{m_j} \sum_{m_l} \langle jlm_j m_l | j l J M \rangle \Upsilon_{lm_l}(\hat{r}_p) \Upsilon_{jm_j}(\hat{R}). \quad (4)$$

The coefficients being the familiar Clebsch–Gordan coefficients. $\Upsilon_{jm_j}(\hat{R})$ and $\Upsilon_{lm_l}(\hat{r}_p)$ are the nuclear rotational and positron angular wavefunctions, respectively. The rotational and positron orbital angular momentum quantum numbers are denoted by j and l , respectively. In this model, $\vec{J} = \vec{j} + \vec{l}$ and its projection M along the nuclear axis are the good quantum numbers (constant of motion of the system).

Using equations (2)–(4) in the Schrödinger equation (1), one gets the corresponding ro-vibrational LFCC coupled differential equation

$$\left(\frac{d^2}{dr_p^2} - \frac{l'(l'+1)}{r_p^2} + k_{\alpha\alpha'}^2 \right) u_{\alpha'}^{Jjl}(r_p) = \sum_{v''} \sum_{j''} \sum_{l''} \times \langle \alpha', J | V'(\vec{r}_p, \vec{R}) | \alpha'', J \rangle u_{\alpha''}^{Jjl}(r_p), \quad (5)$$

where α collectively denotes the quantum numbers v, j, l :

$$V'(\vec{r}_p, \vec{R}) = \int \chi_0(\vec{r}_e, \vec{R}) V_{p-mol}(\vec{r}_p, \vec{r}_e, \vec{R}) \chi_0(\vec{r}_e, \vec{R}) d\vec{r}_e, \quad (6)$$

$$k_{jj'vv'}^2 = 2(E - \varepsilon_{jj'} - \varepsilon_{vv'}), \quad (7)$$

where E is the incident positron energy and $\varepsilon_{jj'}$ and $\varepsilon_{vv'}$ are the energy differences between the rotational levels j and j' and the vibrational levels v and v' , respectively.

The matrix elements in the coupled equations are given by the following relation:

$$\langle v' j' l' | V'(\vec{r}_p, \vec{R}) | v'' j'' l'' \rangle = 2 \int \int \int \phi_{v'}(R) \Upsilon_{j'l'}^{JM*} \times (\hat{r}_p, \hat{R}) V'(\vec{r}_p, \vec{R}) \phi_{v''}(R) Y_{j''l''}^{JM}(\hat{r}_p, \hat{R}) dR d\hat{R} d\hat{r}_p. \quad (8)$$

Here, the interaction potential has been expanded in terms of the Legendre polynomial as

$$V'(\vec{r}_p, \vec{R}) = \sum_{\lambda} v_{\lambda}(r_p, \vec{R}) P_{\lambda}(\hat{r}_p, \hat{R}). \quad (9)$$

The vibrational wavefunctions of the molecule are calculated using the following differential equations:

$$\left\{ \frac{d^2}{dR^2} + 2\mu(\varepsilon_v - \varepsilon(R)) \right\} \phi_v(R) = 0, \quad (10)$$

where μ is the reduced mass of the molecule and $\varepsilon(R)$ are electronic energies for different nuclear geometries.

The PCOP potential

The interaction potential is composed of two terms. One is the static potential which arises due to the interaction between the projectile (here a positron) and the static target (here a hydrogen molecule), and the other one represents the interaction between the projectile and the distorted target in the presence of the projectile. In the case of a positron as an incident particle, the static potential and the polarization potential play competitive roles due to their respective repulsive and attractive nature. Thus, it is necessary to find a true polarization potential explicitly meant for the positron as a projectile. Such a polarization potential, the so-called positron correlation polarization potential (PCOP), which also

includes short-range dynamical effects in addition to the long-range part of the distortion has already been employed to give reasonable results for both the atom and molecules. The actual details of this model and its modification for the molecule as the target have been discussed by Gianturco *et al* (1997). Here we present a brief discussion of this potential which has been employed in the present calculation.

Using density-functional theory of the electron–positron system, Boronski and Nieminen (1986) presented results on the positron–electron correlation energy as a function of the density parameter r_s defined by the relation $\frac{4}{3}\pi r_s^3 \rho(r) = 1$, where $\rho(r)$ is the undistorted electron density of the target. The positron correlation polarization (PCOP) is derived as a functional derivative of the correlation energy with respect to $\rho(r)$ and its interpolated analytic form is given by the following relation (in atomic units) for $r_s \leq 0.302$:

$$2V_{\text{corr}}(r) = \frac{-1.30}{\sqrt{r_s}} + (0.051 \ln r - 0.115) \ln r_s + 1.167, \quad \text{for } 0.302 \leq r_s \leq 0.562 \quad (11a)$$

$$V_{\text{corr}}(r) = -0.92305 - \frac{0.09098}{r_s^2} \quad \text{and for } 0.56 \leq r_s \leq 8.0 \quad (11b)$$

$$2V_{\text{corr}}(r) = \frac{8.7674r_s}{(r_s + 2.5)^3} + \frac{13.151 + 0.9552r_s}{(r_s + 2.5)^2} + \frac{2.8655}{(r_s + 2.5)} - 0.6298. \quad (11c)$$

This short-range correlation potential is calculated near the target and then matched with the asymptotic form of the polarization potential

$$V_{\text{pol}}(\vec{r}) = -\frac{1}{2r^4}(\alpha_0 + \alpha_2 P_2(\cos \theta)) \quad (12)$$

(α_0 and α_2 are the spherical and non-spherical polarizabilities of the molecule) at the first crossing point. Altogether these form (equations (11) and (12)) the positron correlation polarization (PCOP) potential. It should be noted that the short-range part of this potential is divided by a factor of $(2l + 1)/\sqrt{4\pi}$ to take account of single-centre expansion of the symmetry-adapted angular basis set.

Computational details

Here we have calculated the integrated total, vibrational and rotational excitation cross sections for the positron–hydrogen molecule collision in the lower-energy region of the incident positron. To get the results, the coupled differential equation (5) has been solved using the variable step size Numerov method. The integration has been carried out up to the radial distance of the positron, $100a_0$. The interaction potentials are calculated using the same electronic wavefunction of the hydrogen molecule as used by Gianturco and Mukherjee (1997, 2001) (obtained from the Slater-type orbital (STO) with Gaussian basis set expansions, using the self-consistent field (SCF) results of Dunning (1989)).

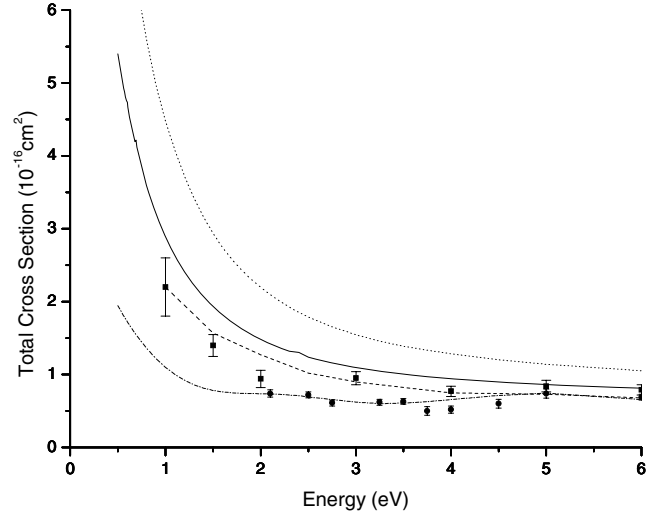


Figure 1. Calculated and measured total integral cross section for positron–hydrogen molecule scattering versus incident positron energy. Solid line: the present ro-vibrational LFCC results, dot line: BFVCC results of Gianturco and Mukherjee (2001), dashed-dot line: ro-vibrational LFCC results of Sur and Ghosh (1985), dashed line: the Schwinger multichannel method of Lino *et al* (1998), filled squares: Hoffman *et al* (1982), filled circles: Charlton *et al* (1983).

This wavefunction gives the value of the electronic ground-state energy of -1.12 Hartree at an inter-nuclear equilibrium distance of 0.73 \AA . The convergent results are obtained using maximum moments for the static potential $\lambda_{\text{max}} = 12$, maximum partial waves $l_{\text{max}} = 8$, maximum rotational states $j_{\text{max}} = 4$, maximum vibrational states $v_{\text{max}} = 4$ and the maximum total quantum number $J_{\text{max}} = 4$. The maximum number of coupled equations solved is 45. In table 1 we have tabulated the vibrational and rotational threshold energies for the hydrogen molecule. To calculate the energies, we need to use the values of the rotational constant $B (= 1/2I)$, where I is the moment of inertia of the molecule) for different vibrational states. Under the B–O approximation applied to the vibrational and rotational motion of the nuclei, we have used a fixed value of B for every rotational and vibrational level.

Results and discussions

In table 2 we have tabulated the (integrated) total and vibrational excitation cross sections for the positron–hydrogen molecule collision in the energy range $0.5\text{--}10.0 \text{ eV}$ of the incident positron energy. In figure 1 we have plotted the present total cross sections with the BFVCC results of Gianturco and Mukherjee (2001), the ro-vibrational results of Sur and Ghosh (1985) and the Schwinger multichannel results of Lino *et al* (1998) along with the measured values of Hoffman *et al* (1982) and Charlton *et al* (1983) below the positronium-formation threshold.

It is evident from figure 1 that the present results agree well with the measured values in the whole energy range below the positronium-formation threshold. However, the results of Lino *et al* are more closer to the measured values of Hoffman *et al* due to an adequate choice of their basis functions to

Table 1. Vibrational and rotational threshold energies (in eV) for the hydrogen molecule. v and j label the vibrational and rotational quantum numbers.

$v = 0$			$v = 1$			$v = 2$			$v = 3$			$v = 4$		
$j = 0$	2	4	0	2	4	0	2	4	0	2	4	0	2	4
0.0	0.05	0.15	0.52	0.56	0.67	1.0	1.05	1.15	1.46	1.5	1.61	1.88	1.93	2.03

Table 2. Vibrational (integrated) elastic and excitation cross sections (in a_0^2) using the ro-vibrational LFCC method for the positron–hydrogen molecule collision. $(-n) \approx 10^{-n}$.

E (eV)	$0 \rightarrow 0$	$0 \rightarrow 1$	$0 \rightarrow 2$	$0 \rightarrow 3$	Total
0.50	19.284				19.284
0.56	17.463	0.135			17.598
0.57	17.258	0.169			17.428
0.58	16.994	0.177			17.171
0.59	16.808	0.183			16.991
0.60	16.721	0.187			16.908
0.61	16.290	0.191			16.480
0.63	15.826	0.195			16.021
0.65	15.361	0.197			15.558
0.67	14.952	0.257			15.209
0.675	14.864	0.224			15.089
0.68	14.780	0.203			14.983
0.69	15.803	0.250			15.053
0.70	14.496	0.213			14.710
0.80	12.648	0.184			12.833
0.90	11.295	0.182			11.477
1.00	10.171	0.149			10.321
1.10	9.253	0.135	0.448(−3)		9.389
1.20	8.482	0.123	0.526(−3)		8.606
1.30	7.832	0.108	0.533(−3)		7.946
1.40	7.279	0.104	0.541(−3)		7.384
1.50	6.804	0.971(−1)	0.503(−3)	0.126(−5)	6.902
1.60	6.395	0.912(−1)	0.608(−3)	0.239(−5)	6.487
1.70	6.039	0.859(−1)	0.452(−3)	0.289(−4)	6.126
1.80	5.729	0.814(−1)	0.406(−3)	0.107(−4)	5.811
1.90	5.457	0.775(−1)	0.409(−3)	0.250(−4)	5.535
2.00	5.217	0.740(−1)	0.369(−3)	0.889(−5)	5.292
2.10	5.005	0.710(−1)	0.341(−3)	0.528(−5)	5.077
2.20	4.817	0.683(−1)	0.323(−3)	0.264(−5)	4.886
2.30	4.649	0.659(−1)	0.312(−3)	0.316(−5)	4.715
2.40	4.499	0.637(−1)	0.302(−3)	0.275(−5)	4.563
2.50	4.364	0.618(−1)	0.290(−3)	0.211(−5)	4.427
2.75	4.082	0.576(−1)	0.272(−3)	0.223(−5)	4.140
3.00	3.860	0.541(−1)	0.259(−3)	0.206(−5)	3.915
3.25	3.684	0.511(−1)	0.250(−3)	0.204(−5)	3.735
3.50	3.540	0.485(−1)	0.244(−3)	0.217(−5)	3.589
3.75	3.421	0.462(−1)	0.240(−3)	0.238(−5)	3.468
4.00	3.322	0.442(−1)	0.237(−3)	0.254(−5)	3.367
4.50	3.165	0.406(−1)	0.234(−3)	0.293(−5)	3.206
5.00	3.046	0.376(−1)	0.232(−3)	0.327(−5)	3.084
6.00	2.873	0.327(−1)	0.227(−3)	0.383(−5)	2.906
7.00	2.747	0.289(−1)	0.220(−3)	0.420(−5)	2.777
8.00	2.648	0.260(−1)	0.213(−3)	0.449(−5)	2.674
9.00	2.565	0.237(−1)	0.206(−3)	0.462(−5)	2.589
10.00	2.492	0.219(−1)	0.199(−3)	0.476(−5)	2.514

account for polarization effects. The figure also shows that the overall shape of the total cross-section energy dependence follow rather closely with the BFVCC result of Gianturco and Mukherjee (2001), the ro-vibrational LFCC result of Sur and Ghosh and the result of Lino *et al.* However, the values of the present calculated cross sections differ with the BFVCC

(which has been obtained with the PCOP potential), the ro-vibrational LFCC results of Sur and Ghosh and the Schwinger multichannel results of Lino *et al.* The larger values of the BFVCC cross sections over both the ro-vibrational LFCC results clearly demonstrate the nature and relative strength of the different coupling schemes.

Sur and Ghosh have compared their ro-vibrational LFCC cross sections with the other results which were obtained using coupled (rotational LFCC) and uncoupled (with a sophisticated polarization potential) schemes and have demonstrated the importance of the inclusion of the effect of vibration in the coupling scheme. Gianturco and Mukherjee (1997) have also described the necessity of the inclusion of the dynamical coupling effect between the positron and the target molecule through the vibrational close coupling method when their results were compared to the measured values.

Gianturco and Mukherjee (1997) have also compared their BFVCC total cross section with the AAMC (adiabatic angular momentum coupling) results and concluded that the ‘... coupling between the positron angular momentum and that of the target via the strongly anisotropic interaction cannot be simplified ...’. They also pointed out that the responsibility for the unrealistic AAMC result lies with the simplification involved in the decoupling scheme through the omission of the geometric factor, which represents the effective coupling between the projectile angular momentum and the electronic angular anisotropy of the charge distribution (mathematically, this means the coupling between l , the projectile orbital angular momentum and λ , the moments of the potential representing the anisotropy of the charge distribution, through the Clebsch–Gordan coefficient), from the coupled potential matrix elements.

Their conclusion is instructive, saying that apart from the target anisotropic factor λ the rotational motion of the nuclei also involves the target anisotropy through the nuclear rotational angular momentum j . Therefore, the rotational coupling effect between the projectile and the target should be taken into account in calculating the scattering parameters. This coupling effect can be included through the rotational close-coupling approximation scheme. The present ro-vibrational LFCC calculation includes this coupling through the angular momentum coupling representation of the total wavefunction (equation (4)). It is to be noted that in the rotational LFCC model the coupling between j , l and λ is included through the Clebsch–Gordan and Racah coefficients in the potential matrix elements.

The present calculated data reflects the effect of this coupling on the total cross section. Figure 1 shows that the rotational coupling effect significantly reduces the higher values of the BFVCC result. This implies that these two

major coupling effects compete with each other and ultimately produce smaller cross sections than the pure vibrational close-coupling results. However, the effect of the rotational coupling decreases with the increase of the energy of the incident positron, as expected. Thus, the difference between the ro-vibrational LFCC results and the vibrational BFVCC results, especially in the low-energy region, clearly shows the importance of the inclusion of the rotational motion in a dynamical way along with the vibrational motion.

Furthermore, figure 1 shows that there is also a marked difference between the present ro-vibrational LFCC total cross section with the ro-vibrational LFCC result of Sur and Ghosh (1985) below 4.0 eV. This difference may be attributed to the following two reasons. The main reason behind this is the use of a different polarization potential in the calculations. It was mentioned above that the polarization potential plays a key role in positron scattering as its attractive nature opposes the repulsive nature of the static potential which tend to cancel each other. In the present calculation, we have used a better parameter-free model positron correlation polarization (PCOP) potential with specific positron signature in comparison to the polarization potential used by Sur and Ghosh, which does not include any positron signature. As the present calculation includes a better polarization potential, the present result is expected to be more reliable and therefore the calculated data very closely agree with the measured data near the low-energy region where the polarization potential plays a predominant role.

The other reason behind the difference in the result between the two ro-vibrational methods is the use of two different target electronic wavefunctions mentioned earlier; the wavefunction used by Sur and Ghosh is simpler. Therefore, as far as the target wavefunction is concerned the present result is more reliable. Thus, it may be concluded from the above discussions that the present ro-vibrational LFCC calculation predicts a reliable estimate of the total cross section for positron–hydrogen molecule scattering in the energy region considered.

In figures 2 and 3, we have plotted the present $v = 0 \rightarrow v = 1$ and $v = 0 \rightarrow v = 2$ vibrational excitation cross sections along with the BFVCC result of Gianturco and Mukherjee (2001), where the magnitude of $v = 0 \rightarrow v = 2$ is very small. In figure 2, we have also included the ro-vibrational LFCC result of Sur and Ghosh (1985) and the measured values of Sullivan *et al* (2001). It is seen that although the overall nature of the change of these inelastic cross sections with energy is similar except near the threshold region, the absolute values of the cross sections differ. The reason for the larger values of BFVCC cross sections over the present ro-vibrational LFCC results is similar to the above discussions made about total cross sections. But the result of Sur and Ghosh for $v = 0 \rightarrow v = 1$ behaves differently when compared to the present result; it is larger. The polarization potential used by Sur and Ghosh is weaker than the PCOP potential giving smaller values of total cross section as is evident from figure 1. The value of the total cross section is dominated by elastic cross section as shown in table 2. Thus, the variation of the total cross section using two different polarization potentials mainly

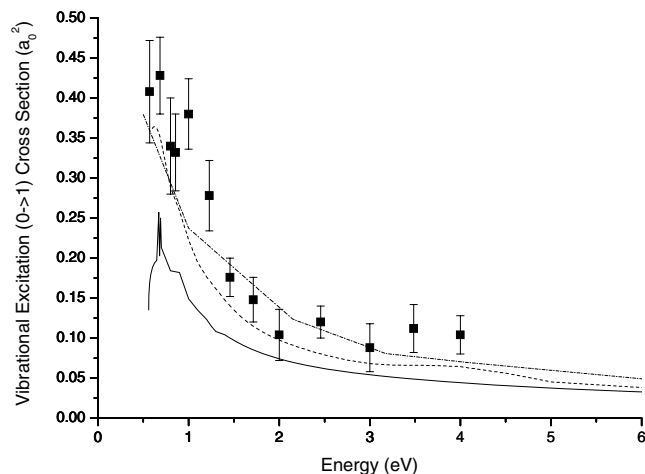


Figure 2. Calculated and measured partial integral vibrational ($0 \rightarrow 1$) cross section for positron–hydrogen molecule scattering versus incident positron energy. Solid line: the present ro-vibrational LFCC results, dashed line: BFVCC results of Gianturco and Mukherjee (2001), dashed-dot line: ro-vibrational LFCC results of Sur and Ghosh (1985), filled squares: Sullivan *et al* (2001).

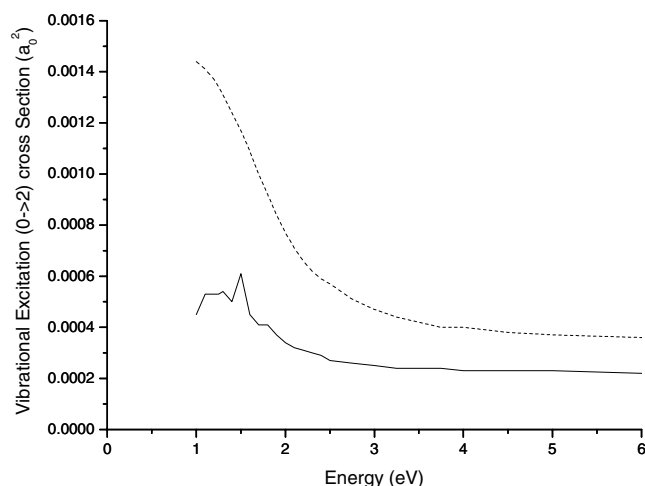


Figure 3. Calculated partial integral vibrational excitation ($0 \rightarrow 2$) cross section for positron–hydrogen molecule scattering versus incident positron energy. Solid line: the present ro-vibrational LFCC results, dashed line: ro-vibrational LFCC results of Sur and Ghosh (1985).

reflects the change of elastic cross section. Thus, it seems apparent from figures 1 and 2 that the polarization potential acts oppositely to the elastic and excitation processes.

At this point, it is important to note that unlike the electron, the positron is distinguishable from the target electrons. As the positron penetrates the region occupied by the electrons, details of its effect on the molecular wavefunctions remain important. Thus, a good and elaborate target molecular electronic wavefunction should be used to get better estimates of the scattering parameters. Sur and Ghosh have used a simple target electronic wavefunction, which may be the reason for the different behaviour of the inelastic cross section.

Furthermore, from figures 2 and 3, it is seen that the present excitation cross sections have structures near the

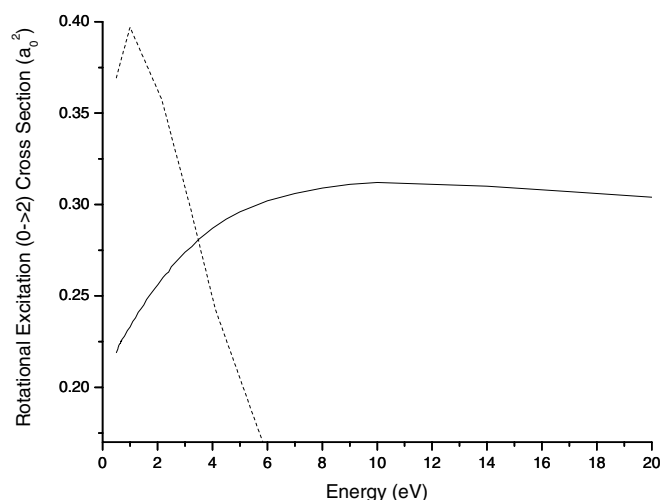


Figure 4. Calculated partial integral rotational excitation ($0 \rightarrow 2$) cross section for positron–hydrogen molecule scattering versus incident positron energy. Solid line: the present ro-vibrational LFCC results, dashed line: ro-vibrational LFCC results of Sur and Ghosh (1985).

inelastic thresholds, whereas the other results show smooth variation. It is interesting to note that the measured values also show structure-like behaviour in the low-energy region.

It is also to be noted that although all the theoretical results, as shown in figure 2, follow well the shape of the measurement, so far as the absolute values are concerned the present ro-vibrational LFCC values differ marginally with the measured values. To remove this discrepancy, we feel that more work should be done for this system.

Figure 4 shows the present $j = 0 \rightarrow j = 2$ rotational excitation cross section for the vibrational ground state along with the result of Sur and Ghosh. To see the nature of the variation of this inelastic cross section with energy, we have calculated and have plotted the values up to 20 eV, although in the higher part of the considered energy region the other inelastic channels are open and the rotational effect is negligible. The present result shows that the cross section first increases with energy up to 10.0 eV and then slowly decreases. However, the cross section calculated by Sur and Ghosh shows different behaviour. The overall variation of the present result is smooth and systematic in contrast to the result of Sur and Ghosh. This different behaviour may also be attributed to the use of a different polarization potential and different target electronic wavefunction in the two calculations.

Conclusion

In this work, we have presented a theoretical calculation of the positron–hydrogen molecule collision using the ro-vibrational laboratory frame close-coupling (ro-vibrational LFCC) scheme under the Born–Oppenheimer approximation in the low-energy region of the incident positron. To calculate the scattering parameters, we have used an efficient positron correlation polarization (PCOP) potential obtained especially

with a positron as the incident particle. We have compared our results with the measured values and with the other theoretically calculated data.

The present total cross section agrees well with the measured data. However, we have found that there are differences in results among the theoretical predictions. The difference of the present total cross section with the body-frame vibrational close coupling (BFVCC) result is attributed to the inclusion of the effect of rotational coupling on the scattering process. However, the dissimilarity of the present result with the existing ro-vibrational LFCC calculation (using a parameter-dependent polarization potential), especially in the very low-energy region, and the Schwinger multichannel result is mainly due to the use of different kinds of polarization potential. The suitability of a model potential can be verified when it is used to calculate the total cross section in scattering phenomena. From the above discussions, we can say that the PCOP potential may be used to predict a good theoretical estimate of the total cross section for positron scattering.

We have also compared the present vibrational and rotational excitation cross sections with the other results. These results also show the effect of the rotational and vibrational coupling in the dynamics of the scattering process.

Finally, we conclude that to obtain reliable estimates of the scattering parameters in positron molecule scattering, one should consider the dynamics of the rotational and vibrational motion in the coupling scheme, and also use a good model polarization potential. It seems likely that this will also hold for other molecules, but calculations should be performed to check this.

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References

- Armour E A G 1988 *Phys. Rep.* **169** 1
- Boronski E and Nieminen R M 1986 *Phys. Rev. B* **34** 3820
- Charlton N, Griffith T C, Heyland G R and Wright G L 1983 *J. Phys. B: At. Mol. Phys.* **16** 323
- Dunning T M 1989 *J. Chem. Phys.* **90** 1007
- Ghosh A S and Mukherjee T 1996 *Can. J. Phys.* **74** 420
- Ghosh A S, Mukherjee T, Biswas P K and Jain A 1993 *J. Phys. B: At. Mol. Opt. Phys.* **26** L23
- Gianturco F A and Mukherjee T 1997 *Phys. Rev. A* **55** 1044
- Gianturco F A and Mukherjee T 2001 *Phys. Rev. A* **64** 024703
- Gianturco F A, Mukherjee T and Paoletti P J A 1997 *Phys. Rev. A* **56** 3638
- Henry R J W and Lane N F 1969 *Phys. Rev.* **183** 221
- Hoffman K S, Dababneh M S, Heish Y F, Kauppila W E, Pol V, Smart J H and Stein T S 1982 *Phys. Rev. A* **25** 1393
- Lino J L S, Germano E S, da Silva E P and Lima M A P 1998 *Phys. Rev. A* **58** 3502
- Sullivan J P, Gilbert S J and Surko C M 2001 *Phys. Rev. Lett.* **86** 128
- Sur S and Ghosh A S 1985 *J. Phys. B: At. Mol. Phys.* **18** L715