

Bound state in positron scattering by alleneAlessandra Souza Barbosa,^{*} Sergio d'Almeida Sanchez,[†] and Márcio H. F. Bettega[‡]*Departamento de Física, Universidade Federal do Paraná, Caixa Postal 19044, 81531-990 Curitiba, Paraná, Brazil*

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We report integral and differential cross sections for positron collisions with allene, calculated with the Schwinger multichannel method. The cross sections were computed in the static-polarization approximation for energies up to 7 eV. We have tested a series of single-particle basis sets and different polarization schemes to improve the description of low-energy positron scattering by the allene molecule. We have found that the use of extra centers with no net charge with additional single-particle *s*- and *p*-type functions centered at them are essential in order to accurately reproduce the polarization potential and, hence, obtain proper scattering cross sections. The choice of the allene molecule was due to the fact that it is a highly symmetric molecule with no permanent dipole moment and would allow several different calculations. Our cross sections are compared to the available experimental data for the total cross section with a reasonable agreement after correcting their results due to the low angular discrimination of their apparatus. Also, a virtual state was observed in the integral cross section that became a bound state when the description of the polarization potential is improved. We also observed a Ramsauer-Townsend minimum in the cross section whose location varies from 2.7 to 3.4 eV, depending on the polarization scheme used in the calculations.

DOI: [10.1103/PhysRevA.96.062706](https://doi.org/10.1103/PhysRevA.96.062706)**I. INTRODUCTION**

The interest in positron collision with molecules has greatly increased in recent years with the advent of better experimental equipment, theoretical methodologies, and computers to perform the simulations (see Refs. [1–3] for a recent review). However, there are intrinsic problems in dealing with positron scattering that make such calculations a hard task. In particular, besides the inelastic processes such as electronic excitation and ionization already observed in scattering by different projectiles (such as electrons), the positron can “capture” one of the electrons of the target, forming the positronium (Ps). The positronium formation in positron-molecule collision can be responsible for a large part of the total cross section (TCS) above the positronium formation threshold E_{Ps} [4].

One could expect, on the other hand, that below E_{Ps} , positron scattering would be a task no more difficult to solve than electron scattering, for instance, but this is not the case. By simple arguments using the Gauss law, it is not hard to realize that if the electronic cloud is held frozen throughout the scattering process (the so-called static approximation), the positron would experience a repulsive potential. However, in a collision of a very low-energy positron with molecules (typically below 5 eV), there is enough time for the electronic cloud to distort, creating an induced dipole and a net attractive potential (resulting from the combination of the static and polarization potentials) for the incoming positron. Hence, the correct description of the polarization potential for positron scattering is a hard task for theoreticians.

On the experimental side, positron scattering represents several challenges and only a few groups actually report cross sections for such a process (see Ref. [3] for recommended cross sections for several molecules and processes, such as elastic

and inelastic scattering, ionization, positronium formation, etc). These experimental data, however, do not always agree with each other. To be more specific, recent experiments for positron scattering by methane [5] at very low-energy show a distinct behavior from previously published data. Further analysis has shown that the angular discrimination of the apparatus used by the Japanese group was responsible for such differences, showing the importance of extra measurements in this field [3].

Regarding the comparison between theory and experiment, it is even harder to reach a consensus. Recently, several papers that combined theory and experiments in positron scattering were published [5–10]. In these works, even though there is a qualitative agreement between theory and experiment at energies below E_{Ps} , the experimental data can be much higher than the theoretical results, probably due to problems in correctly treating the polarization potential in these calculations. This can change significantly also according to the experimental apparatus, making the measured data much lower than the calculated one. The annihilation data could indicate, at some energies, if this discrepancy is in fact a theoretical issue.

Several experiments [11–14] were performed on annihilation rates using thermal positrons and a focused beam of positrons on several molecules. They measured the so-called annihilation parameter, or Z_{eff} , which is a dimensionless number proportional to the annihilation rate. In fact, it can also be viewed as a measurement of positron-molecule interaction, since if no interaction is taken into account, $Z_{\text{eff}} = Z$, where Z is the number of electrons in the target. However, usually Z_{eff} is orders of magnitude higher than Z . Some theories were developed [14–17] in order to understand the high annihilation rate measured values. Particularly, if the positron is somehow captured by the target, for instance, in a bound state, it is expected that the probability of annihilation (and, hence, the Z_{eff}) increases. Some scattering calculations predicted virtual states [5,6,18], while other types of calculations [19] actually predicted bound states for positrons' interaction with molecules. In a review published in 2010 [14], Gribakin and

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co-workers reinforced the fact that if a scattering calculation could actually find a positron bound state it would be a major advance for understanding resonant positron annihilation.

In this work, we performed low-energy positron scattering by allene. The choice of target was made because it is a simple molecule, with no permanent dipole moment, and symmetric enough that it would allow us to perform a series of sophisticated scattering calculations. We used the Schwinger multichannel method to calculate integral and differential cross sections using a diverse scheme of single-particle basis and additional functions located in extra chargeless centers. Recently we have shown that the inclusion of extra functions in chargeless centers improves the description of the polarization effects in positron-silane scattering [20]. We compared our results with the only available experimental data measured by Makochekanwa *et al.* [21], which reported total cross section for electron and positron scattering by C_3H_4 molecules. Unfortunately, no experiments on the annihilation parameter were found in the literature for such a target. In a recent publication on recommended cross sections for scattering of positrons by several targets, Brunger and co-workers [3] pointed out the lack of experimental data and theoretical results for several molecules, including allene.

The outline of this paper is as follows: in Sec. II we discuss the SMC method for positron scattering, and we show the computational procedures used in these calculations; in Sec. III we discuss the results obtained for the allene molecules using different basis sets. Then we finish the paper with some conclusions in Sec. IV.

II. THEORY AND COMPUTATIONAL PROCEDURES

The calculations were performed using the Schwinger multichannel method, which is an *ab initio* variational method for the scattering amplitude. This method has been described in detail in several publications [22,23], so here we will discuss only those points that are relevant to the present calculations.

The working expression for the scattering amplitude is

$$f(\vec{k}_f, \vec{k}_i) = -\frac{1}{2\pi} \sum_{m,n} \langle S_{\vec{k}_f} | V | \chi_m \rangle (d^{-1})_{mn} \langle \chi_n | V | S_{\vec{k}_i} \rangle \quad (1)$$

where

$$d_{mn} = \langle \chi_m | A^{(+)} | \chi_n \rangle \quad (2)$$

and

$$A^{(+)} = Q \hat{H} Q + PVP - VG_p^{(+)}V. \quad (3)$$

In the above equations, $|S_{\vec{k}_i, f}\rangle$ is a solution of the unperturbed Hamiltonian H_0 (the kinetic energy of the incoming positron plus the target Hamiltonian) and is a product of a target state and a plane wave, V is the interaction potential between the incident positron and the electrons and nuclei of the target, $|\chi_m\rangle$ is a set of $(N+1)$ -particle configuration state functions (CSFs) used in the expansion of the trial scattering wave function, $\hat{H} = E - H$ is the collision energy minus the full Hamiltonian of the system ($H = H_0 + V$), P is a projection operator onto the open-channel space defined by the target eigenfunctions, and $G_p^{(+)}$ is the free-particle Green's

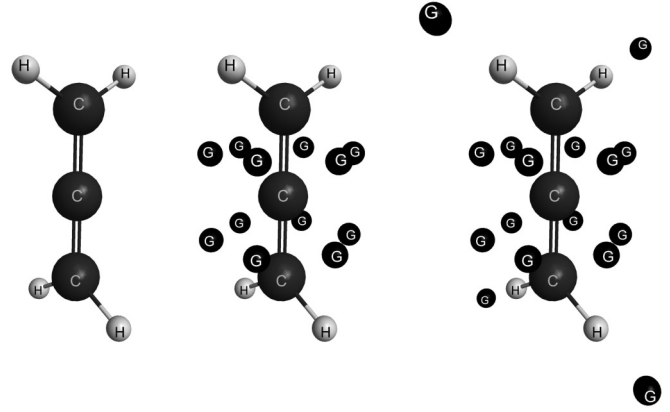


FIG. 1. Geometrical structure of allene molecule with the 12 and 16 extra chargeless centers employed in the calculations.

function projected onto the P space. Finally $Q = (\mathbb{1} - P)$ is the projector onto the closed electronic channels of the target.

The direct space, in the static plus polarization approximation, is composed of CSFs of the form

$$|\chi_{ij}\rangle = |\Phi_1\rangle \otimes |\varphi_j\rangle \oplus |\Phi_i\rangle \otimes |\varphi_j\rangle, \quad (4)$$

where $|\Phi_1\rangle$ represents the ground state of the molecule obtained at the Hartree-Fock (HF) level and $|\varphi_j\rangle$ is a single-particle orbital used to expand the positron scattering orbital (see below). $|\Phi_i\rangle$ is obtained from single virtual excitations of the target out of the HF reference state, from the hole (occupied) orbitals to the particle (unoccupied) orbitals.

The allene molecule belongs to the D_{2d} symmetry group. However, since the SMC method deals only with Abelian groups, we treated the molecule as the C_{2v} symmetry, which irreducible representations are A_1 , A_2 , B_1 , and B_2 . The calculations were performed in the experimental equilibrium geometry of the target, in which the distances between the atoms are $r_{CC} = 1.308 \text{ \AA}$ and $r_{CH} = 1.087 \text{ \AA}$ [24].

The calculations were performed in the static plus polarization approximation, in order to account for the distortion of the electronic cloud due to the incoming positron. In all the calculations performed in this work, we used modified virtual orbitals (MVOs) [25] as particle and scattering orbitals. All 11 valence orbitals were used in the calculations as hole orbitals and also as scattering orbitals.

To perform the scattering calculations we tested several different basis sets. We started with the $6 - 311 + + (3d, 1p)$ as implemented in GAMESS [26]. This resulted in 180/133 (primitives/contracted) Gaussian functions. We then included 12 extra chargeless centers keeping the C_{2v} symmetry of the target. The extra centers were placed in the vertices of two hexagons, of side 1.1 \AA , lying in planes perpendicular to the molecular axis, at half distance from each carbon atom, as shown in Fig. 1. On these centers we placed one s - and one p -type functions, with exponents 0.144 and 0.200, respectively. We also included four more extra centers along the C-H bonds as shown in Fig. 1, in a total of 16 extra centers, also with one s - and one p -type functions with same exponents.

In order to make the discussion of the results clear, all calculations will be named henceforth. The calculation with

TABLE I. Details of the calculations carried out for positron scattering by allene. For each calculation labeled as SP-1 to SP-6 we provide the number of extra centers employed, number of MVOs and number of configuration state functions in A_1 and B_2 symmetry, and the total number of CSFs where applicable.

| Label | Centers | MVOs | A_1 | B_2 | Total CSFs |
|-------|---------|------|--------|--------|------------|
| SP-1 | 0 | 65 | 11 326 | 9 908 | 39 653 |
| SP-2 | 0 | 78 | 15 429 | 13 912 | |
| SP-3 | 12 | 65 | 10 698 | 10 000 | 39 701 |
| SP-4 | 12 | 78 | 14 954 | 14 016 | 55 717 |
| SP-5 | 16 | 65 | 10 868 | 10 004 | |
| SP-6 | 16 | 78 | 15 049 | 14 118 | |

no extra center that used the lowest 65 MVOs [25] as particle orbitals will be labeled SP-1; the same type of calculation, but using the lowest 78 MVOs, will be labeled SP-2; the calculation that included 12 extra centers and used the lowest 65 MVOs will be labeled SP-3; the calculation with 12 extra centers but using the lowest 78 MVOs will be labeled SP-4; the calculation with 16 extra centers and the lowest 65 MVOs will be labeled SP-5; and the calculation with 16 extra centers and 78 MVOs will be labeled SP-6. We highlight that due the high computational effort, we performed calculations only for A_1 and B_2 symmetries employing all schemes, whereas the complete calculation was performed only for SP-1, SP-3 and SP-4 schemes. The nomenclature, basis set types, number of MVOs used as particle and scattering orbitals, and total number of CSFs for each calculation are summarized in Table I. In this sense, our main goal was to investigate the importance of extra functions and/or more CSFs in the description of polarization effects.

III. RESULTS AND DISCUSSION

Since the major difficulty in performing positron scattering calculations is in the low-energy regime, we first performed all the calculations for the totally symmetric irreducible representation A_1 . This is mainly because the contribution of the s -type wave, which is dominant due to no angular momentum barrier, is in this symmetry. In Fig. 2 we plotted the s -wave cross section (top panel) and the s -wave eigenphase (bottom panel). Three main features can be readily observed in this figure: the rapid increase of the cross section as the energy tends to zero, the increase of the eigenphase in this same energy region, and the presence of a Ramsauer-Townsend (RT) minimum [27]. This last feature can be more easily discussed. The net potential felt by the incoming positron is combination of the repulsive static potential and the attractive polarization potential [28]. These two contributions cancel each other at some particular energy, where the s -eigenphase changes sign from positive to negative (the net potential changes from attractive to repulsive), crossing zero, and where the s -wave cross section is zero. Even though a minimum is observed in the $l = 0$ -partial wave cross section, it does not reflect in the total cross section (and is not seen in the experimental data) due to the contribution of higher partial waves at this energy (as shown in Fig. 4).

When we compare the position of the RT minimum, it is located at 2.7 eV for the SP-1 calculation, which employed

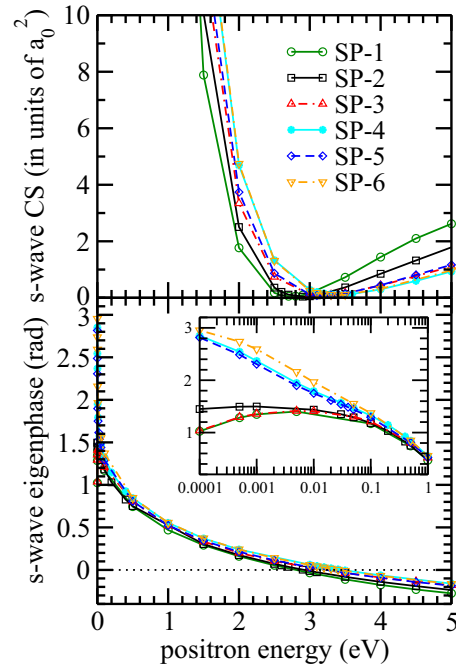


FIG. 2. s -wave cross section (top) and respective eigenphase (bottom) calculated employing different schemes to account for the polarization effects of the molecular electronic cloud due to the incoming positron. The inset presents the same data within a logarithmic energy scale, in order to highlight their very low-energy behavior.

the simplest base and the lowest number of CSFs. As we increase the number of CSFs, the RT minimum shifts to higher energies, as expected [27]. For SP-2, where a better description of the polarization potential is performed, the RT minimum is located at 2.9 eV. This process continues as we include extra centers, and the RT minimum is located at 3.2 eV for SP-3. The inclusion of further CSFs in SP-4 moves the minimum to 3.4 eV. For SP-5, with four more extra centers and the use of only 65 MVOs, the minimum shifts slightly to the left with respect to SP-4 and is located at 3.3 eV. It seems finally converged at 3.4 eV in SP-6. It appears that the inclusion of 12 centers and 78 MVOs as particle orbitals would suffice to describe the scattering process within this basis set.

The first and second features can be analyzed as one, since the same physical phenomenon is responsible for both. The rise in the cross section and in the eigenphase could be due either to a virtual state or to a bound state. If it is a virtual state, the eigenphase goes to $\pi/2$ as the energy goes to zero, and if it is a bound state it goes to π [27]. Another way to differentiate the bound state from virtual state is through the the scattering length (SL), which can be calculated as [27]

$$SL = - \lim_{k \rightarrow 0} \frac{1}{k} \tan \delta_0(k) \quad (5)$$

in which δ_0 is the s -wave eigenphase and k is the momentum of the projectile.

For the SP-1, SP-2, and SP-3 calculations, we observe a very negative scattering length which characterizes a virtual state (ideally it would be minus infinity). In particular, for the SP-2 calculation, we obtained a SL equal to $-3355.6 a_0$.

TABLE II. Scattering length (SL) and Ramsauer-Townsend minimum (R-T min.) position for each calculation.

| Label | SL (a_0) | R-T min. (eV) |
|-------|--------------|---------------|
| SP-1 | -127.2 | 2.7 |
| SP-2 | -3355.6 | 2.9 |
| SP-3 | -637.1 | 3.2 |
| SP-4 | +110.2 | 3.4 |
| SP-5 | +220.2 | 3.3 |
| SP-6 | +69.9 | 3.4 |

By either adding extra centers or more CSFs, the virtual state becomes a bound state for SP-4, SP-5, and SP-6 calculations, which can be verified by the large positive SL. All the results discussed here are summarized in Table II.

These results confirm the importance of the use of extra centers and an appropriate configuration space in the polarization calculations. It is well known that, as the interaction potential between the target and the projectile becomes more and more attractive, the RT minimum shifts to higher energy. As it appears, with the basis set employed in this calculation, we have reached convergence in SP-4, with the position of the minimum at 3.4 eV. The fact that the virtual state becomes bound as the polarization calculation becomes better described may be the key to understand high annihilation rates observed in positron scattering by molecules. Experiments have shown [11–14] in both thermal positrons and beam experiments that the Z_{eff} obtained is much higher than the number of electrons in the target, which indicates a high interaction of the incoming positron with the molecule. The present theoretical models [14–17] also indicate that the presence of a bound state would be important in understanding annihilation rates, particularly in the beam experiments. So far, there are several calculations of positron binding energies by molecules, but, to the best of our knowledge, a bound state in fixed nuclei scattering calculations has not been observed so far. The only other result in which a bound state was observed in scattering calculations was in positron collision with acetylene when nuclear dynamics was considered [29].

Unfortunately, there are no experimental data on positron annihilation by allene. Hence, there is no experimental evidence that a positron can attach to allene. However, if we consider similar molecules in which we have experimental data, a bound state is expected even though the calculations performed indicated only a virtual state [6,18]. This difference could be due to the lack of extra centers or a large enough number of CSFs in the previous calculations.

In Fig. 3 we also plot the results for all basis sets for the A_1 and B_2 symmetries. Since there is degeneracy between B_2 and B_1 irreducible representations, and the A_2 symmetry does not contribute much to the integral cross section, we focused our attention only on the A_1 and B_2 symmetries. The same behavior of the s -wave cross section displayed in Fig. 2 can be seen in the A_1 ICS. For the B_2 cross section, we can clearly see the effect of the angular momentum barrier as the ICS starts at zero and grows as the energy increases, having a peak around 1.5 eV. The difference in the peak height may also indicate the need of a flexible enough single-particle basis set either by increasing the number of extra centers and of the number

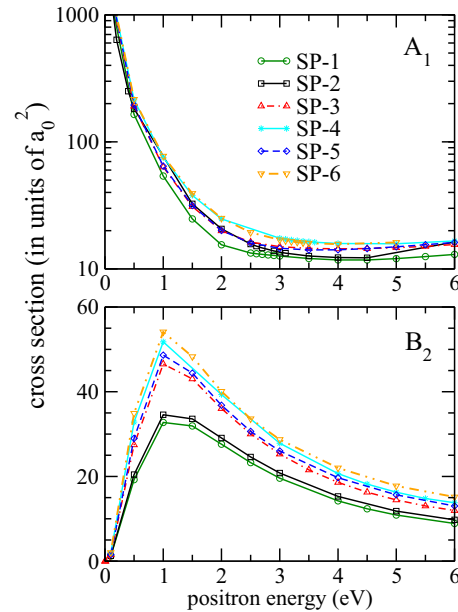


FIG. 3. A_1 and B_2 components of the integral cross sections for positron scattering by allene, obtained employing different schemes to account for the polarization effects of the molecular electronic cloud due to the incoming positron.

of CSFs, as was discussed in Ref. [30]. In that work, it was shown that a better representation of the effect of the angular momentum barrier may be important to make the total ICS higher in magnitude and, hence, better describe the correct

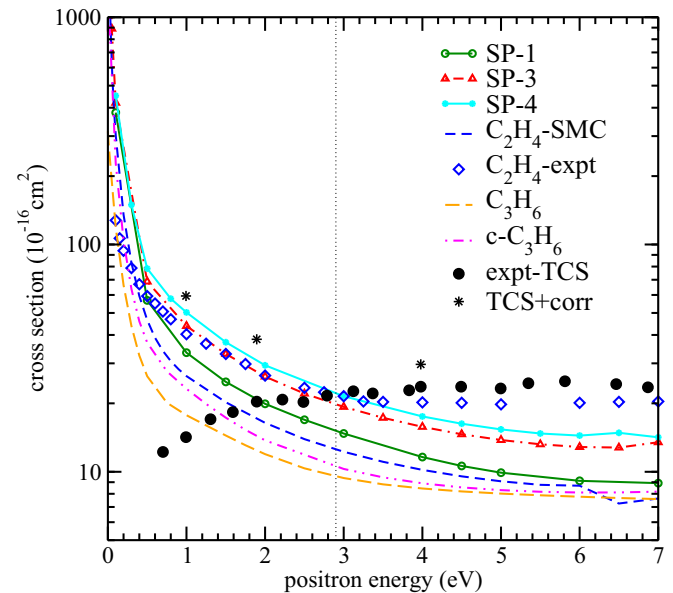


FIG. 4. Present integral cross section for elastic positron scattering by allene obtained in the SP-1, SP-3, and SP-4 approximations. The calculated cross sections are compared with the available experimental total cross sections (expt-SCT) [21] for allene, calculated ICSs and experimental TCS for ethene (C_2H_4) [6], and calculated ICSs for C_3H_6 isomers [8]. The vertical line indicates the positronium energy threshold. We also present an estimate for the correction of the experimental TCS (TCS+corr).

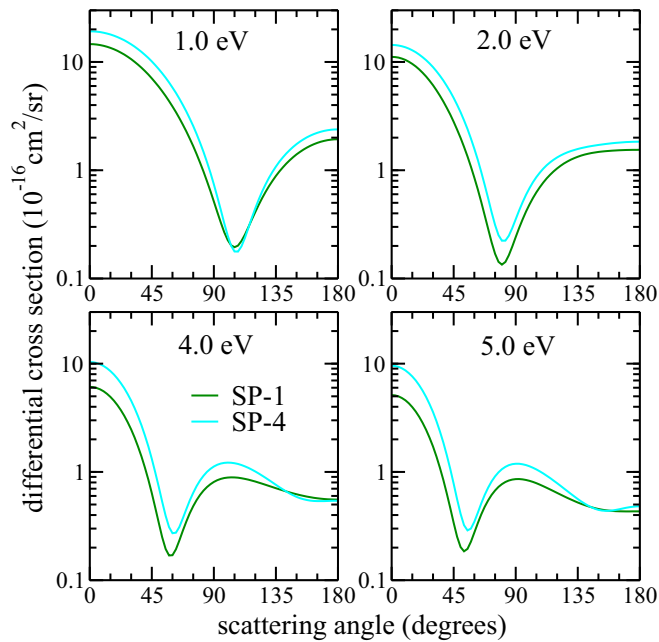


FIG. 5. Present differential cross section for elastic positron scattering by allene obtained in the SP-1 and SP-4 approximations at 1.0, 2.0, 4.0, and 5.0 eV.

scattering process. By these standards, the best results shown in the Fig. 3 are from SP-4 and SP-6 calculations.

Finally, we present, in Fig. 4, the integral cross section for the SP-1, SP-3, and SP-4 calculations in comparison with the only available experimental data for the allene molecule from Makochekanwa *et al.* [21]. We can see a big discrepancy from our calculated ICS and the experimental TCS, not only in magnitude but also especially in tendency at very low energy. This discrepancy is not really something to worry or unheard, since it had already appeared in many systems prior to this work [5–8]. It is due to a poor angular discrimination of the experimental apparatus. As a way to better understand this, we have included the experimental data for the ethene molecule from the Trento group [6], which have a better experimental setup. It shows the same feature as our calculations at very low energy. Since the Japanese group did not report the angular discrimination of their apparatus, we employed the missing angles reported by Ref. [31], in order to estimate the correction to the experimental data. Our calculated DCSs, obtained in the SP-4 approximation (shown in Fig. 5), were used for this purpose. It becomes clear from this point that our calculated

cross section shows now the same qualitative behavior as the corrected measured TCS. It is important also to notice in this figure that the inclusion of extra centers and the large number of CSFs increase the magnitude of our calculated ICS. This can also be seen when compared to our previous calculation for the C_3H_6 [8] molecule with no extra center. Even though propene is a bigger molecule than allene and has a small dipole moment (0.366 D [32]), the calculated ICS was even lower than the ones performed in this work.

In Fig. 5 we present calculated differential cross sections at 1.0 eV, 2.0 eV, 4.0 eV, and 5.0 eV for the SP-1 and SP-4 calculations. All the curves show approximately the same behavior but differ in magnitude, specially at lower angles, with SP-4 being higher than SP-1.

IV. CONCLUSIONS

We have calculated integral and differential cross sections for positron scattering by allene with different polarization schemes, with and without the inclusion of extra centers. From our calculations, we found that the virtual state observed in SP-1, SP-2, and SP-3 calculations becomes bound by increasing either the number of particle and scattering orbitals or the number of extra centers in the calculation, as seen in SP-4, SP-5, and SP-6 data. This is important since a bound state was not previously obtained in any scattering calculations, even though some models for positron annihilation predict its existence. We also showed how a good description of the polarization potential by including extra centers and by constructing an appropriate configuration space can be important in other symmetries, as to better represent the effect of angular momentum barrier, bringing the total ICS to higher values. This is also shown when we compared our calculations with the corrected experimental data for the forward angle scattering using our calculated DCSs. In this case a good agreement was found between the SP-4 calculation and the corrected total cross section.

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