Elastic positron scattering by C_2H_2: Differential cross sections and virtual state formation

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We present calculated elastic differential cross sections for positron-acetylene scattering, obtained by using the Schwinger multichannel method. Our results are in very good agreement with quasielastic experimental data of Kauppila *et al.* [Nucl. Instrum. Meth. Phys. Res. B **192**, 162 (2002)]. We also discuss the existence of a virtual state (zero-energy resonance) in e^+-C_2H_2 collisions, based on the behavior of the integral cross section and of the *s*-wave phase shift. As expected the fixed-nuclei cross section and annihilation parameter (Z_{eff}) present the same energy dependence at very low impact energies. As the virtual state energy approaches zero, the magnitude of both cross section and Z_{eff} are extremely enhanced (at zero impact energy). The possibility of shifting from a low-lying virtual state to a shallow bound state is not expected to significantly affect room-temperature annihilation rates.

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I. INTRODUCTION

In recent years, a few different pathways have been proposed to account for very high annihilation rates observed for several polyatomic gases [1], such as formation of virtual states [2], formation of virtual positronium followed by pick-off annihilation (i.e., with one of the *other* molecular electrons) [3], nonresonant vibrational coupling [4,5], and vibrational Feshbach resonances [6]. Nevertheless, this matter remains controversial and the dynamical features of the annihilation process are not fully understood. The relevance of virtual state formation in the annihilation dynamics was originally pointed out by Paul and Saint-Pierre [2], who performed a model calculation for CH_4. The existence of virtual states is theoretically well established for atomic systems [7], but polyatomic molecules lack for similar studies.

On the other hand, quite significant experimental progress was achieved in recent years [1,8–10] and, particularly, measurements of quasielastic differential cross sections (DCS) for positron scattering are now available [11]. The DCS are quasielastic because the energy resolution of the positron beam is not good enough for distinguishing rotationally and vibrationally inelastic scattering from the electronically elastic DCS. Despite this limitation, such measurements are a significant progress because they may help to remedy the lack of experimental data in the field. More recently, DCS were obtained for CO_2 [12–14], O_2 [13,14], N_2, CO, and N_2O [14] and also for C_2H_2 and SF_6 [15].

In view of these facts, acetylene happens to be a very interesting system. First, its experimental annihilation rate is quite large, $Z_{\text{eff}}=3160$ [16] though $Z=14$, thus being a prototype system for a theoretical investigation on annihilation dynamics. Acetylene and nitrogen are also isoelectronic, the latter being used as a buffer gas in experimental devices due to its low annihilation rate (average experimental Z_{eff} value about 30 [16]), among other aspects. Moreover, the existence of a e^+-C_2H_2 virtual state has been considered [17,18], but not fully explored. Finally, experimental quasielastic DCS for this molecule have been reported [15].

In this work, our goals are (i) to compare calculated elastic DCS for acetylene with (quasielastic) experimental data. This was done for nitrogen in a previous work [17]; (ii) to discuss the formation of a virtual state (zero-energy resonance) in e^+-C_2H_2 collisions through estimates of scattering length, comparison with a model box potential calculation, and also through the behavior of both integral cross section (ICS) and *s*-wave phase shifts; (iii) to connect the virtual state formation with the much higher Z_{eff} of acetylene, as compared to nitrogen, through a qualitative analysis. In a recent article [19], we pointed out that our Z_{eff} calculations are underestimated with respect to the experimental data. Despite this, N_2 and C_2H_2, both having $Z=14$, present Z_{eff} curves with strikingly different qualitative behaviors that indicate the influence of virtual state formation.

II. THEORY

The Schwinger multichannel (SMC) method for positron scattering is described elsewhere [20,21] and here we only give the working expression for the scattering amplitude,

$$[f_{\vec{k}_f,\vec{k}_i}]=-\frac{1}{2\pi}\sum_{m,n}\langle S_{\vec{k}_f}|V|\chi_m\rangle(A^{(+)\,-1})_{mn}\langle\chi_n|V|S_{\vec{k}_i}\rangle, \tag{1}$$

with

$$A^{(+)}=Q\hat{H}Q+PVP-VG_P^{(+)}V. \tag{2}$$

In the above expressions, $S_{\vec{k}_{i(f)}}$ is a solution of the unperturbed Hamiltonian (molecular Hamiltonian plus the kinetic energy operator for the incident positron), V is the interaction potential between the incident positron and the molecular target, $|\chi_m\rangle$ is a *configuration* state, i.e., an $(N+1)$-particle variational trial function (the product of a target state and a positron scattering orbital). P and Q are projection operators onto energetically open and closed electronic states of the target, respectively, $\hat{H}$ is the collision energy minus the full scattering Hamiltonian, and $G_P^{(+)}$ is the free-particle Green's function projected on P space.

The SMC scattering wave function is written as

$$|\Psi_{\vec{k}_i}^{(+)}\rangle = \sum_{m,n} |\chi_m\rangle (A^{(+)-1})_{mn} \langle \chi_n | V | S_{\vec{k}_i}\rangle, \tag{3}$$

and may be used for calculating the annihilation parameter (Z_{eff}), which is defined as [22]

$$Z_{\text{eff}}(k_i) = \frac{1}{4\pi} \int d\hat{k}_i \langle \Psi_{\vec{k}_i}^{(+)} | \left[\sum_{j=1}^{Z} \delta(\vec{r}_j - \vec{r}_p) \right] | \Psi_{\vec{k}_i}^{(+)} \rangle. \tag{4}$$

In present calculations, only elastic scattering is considered and one therefore finds $P = |\Phi_0\rangle\langle\Phi_0|$, where $|\Phi_0\rangle$ is the target's ground state. Positron-target interaction may be treated in two levels of approximation, namely static (*S*) and static plus polarization (SP). In the former, the target is kept frozen in its ground state, and the configurations used to expand the trial scattering wave function take the form

$$|\chi_m\rangle = |\Phi_0\rangle \otimes |\varphi_m\rangle, \tag{5}$$

where $|\varphi_m\rangle$ is a positron scattering orbital. SP approximation, on the other hand, takes polarization effects into account through single excitations of the $(N+1)$-particle compound system. The configurations are then given by

$$|\chi_{mn}\rangle = |\Phi_m\rangle \otimes |\varphi_n\rangle, \tag{6}$$

where $|\Phi_m\rangle$ is a singly excited target state.

III. COMPUTATIONAL ASPECTS

Details about the description of the target as well as of correlation effects are given elsewhere [17]. (Present results for acetylene were obtained with the large basis set of Ref. [17].) The target was treated as belonging to the D_{2h} symmetry group and the nuclei were held fixed throughout the collision (fixed-nuclei approximation). Our results took polarization effects into account (SP approximation) amounting to a total of about 45 000 configurations. To our knowledge, this is the most elaborate *ab initio* calculation ever performed for e^+-C_2H_2 scattering.

IV. RESULTS AND DISCUSSION

A. Differential cross section

In Fig. 1 we show our calculated elastic DCS at selected energies. The relative experimental quasielastic data [15] have been normalized to our results at 60 deg. It should be mentioned that our calculations disregarded the positronium (Ps) formation channel, which should be taken into account for energies above ~4.6 eV [23]. Unfortunately, normalization of the experimental data makes it difficult to estimate the effect of neglecting Ps formation. In principle, if the competition between elastic and Ps formation channels was considered, calculated elastic cross sections were expected to present smaller magnitude. Nevertheless, the general agreement is encouraging. The fact that calculations oscillate a little more than experimental data may be due to the quasielastic character of the former, because vibrationally inelastic contributions may hide the structure of purely elastic scattering. The contribution of vibrational excitations to experimental DCS magnitude should also be hidden by the normalization performed. We mention in passing that similar DCS at different impact energies are also available [17].

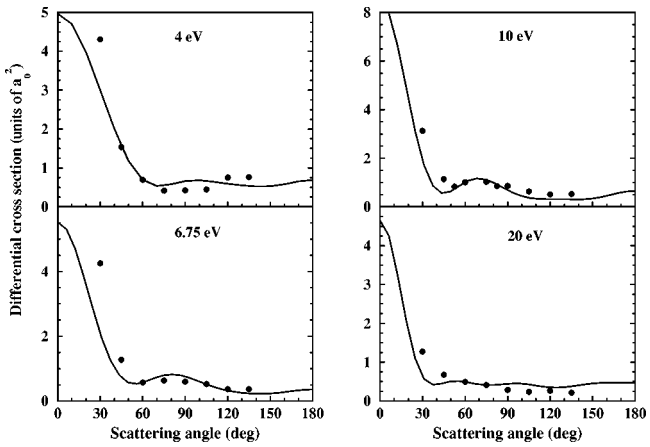

FIG. 1. Elastic differential cross sections (DCS) for e^+-C_2H_2 scattering at 4, 6.75, 10, and 20 eV. Solid line: present results; circles: experimental quasielastic DCS [15].

B. Integral cross section

Occhigrossi and Gianturco [24] have recently reported the elastic integral cross section (ICS) for e^+-acetylene collisions below the Ps formation threshold. Unfortunately, the authors avoided comparison with our previously reported ICS [17]. We believe such comparison would be of help in understanding the difficulties involved in calculations concerning positron scattering by polyatomics, since the two results were obtained with different frameworks. Occhigrossi and Gianturco solved a single-body (potential scattering) problem, in which long- and short-range polarization effects were taken into account through model potentials. The SMC approach, on the other hand, keeps the many-body character of the collision. An accurate description of polarization effects thus depends on the completeness of the variational basis sets.

In Fig. 2 we compare calculated ICS with experimental total cross section of Sueoka and Mori [23]. A very good agreement between our calculations and experimental data is found below the Ps formation threshold. The fact that results of Ref. [24] are systematically underestimated with respect to experiment suggests that the model may lack a thorough

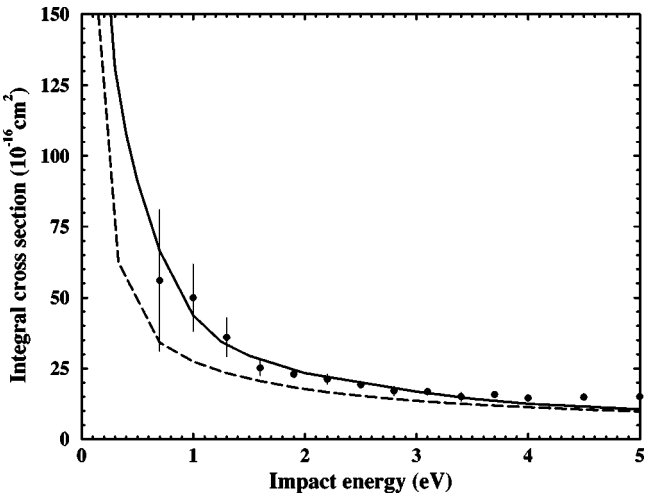

FIG. 2. Elastic integral cross sections for e^+-C_2H_2 scattering. Solid line: present result; dashed line: calculations of Ref. [24]; circles with error bars: experimental data of Ref. [23].

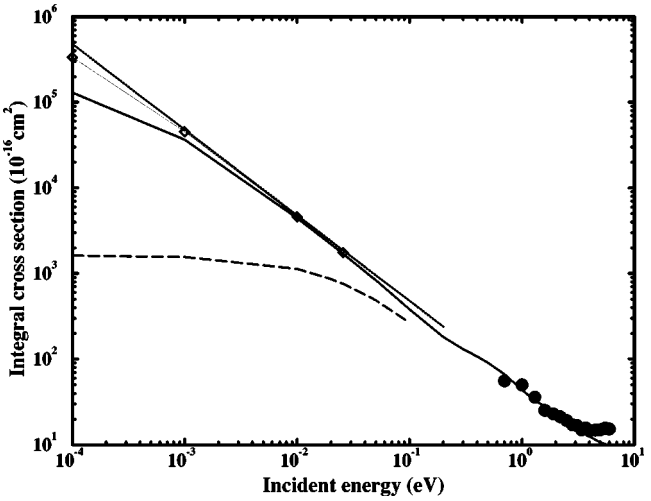

FIG. 3. Integral cross sections for e^+-C_2H_2 scattering. Thick solid line: present result; circles: experimental data of Ref. [23]; dashed line: present result removing the three lowest-lying pseudoeigenstates of the scattering Hamiltonian; dotted line: unitary limit for the *s*-wave cross section; thin solid line with diamonds: present result with augmented configuration space (see text).

description of polarization effects. In Table I we compare molecular polarizabilities and it may be noticed that our basis set provides a very accurate description of both components of the polarizability (agreement with experimental data of Ref. [25] around 1% to 2%). The calculated polarizability of Ref. [24] ($\alpha_\parallel$ component) also compares favorably with experiment (6%). Even though long-range polarization effects often play a relevant role in low-energy collisions, we believe that the difference in calculated polarizabilities may not be enough to account for the big discrepancies observed between our results and those of Ref. [24] below 1 eV. We believe that virtual state (zero-energy resonance) formation takes place in e^+-C_2H_2 collisions (see discussion below), thus requiring a thorough description of both short- and long-range polarization effects.

The behavior of present ICS at very low impact energies is presented in Fig. 3. For the time being, we turn attention to a very interesting qualitative aspect: while ICS for acetylene (Fig. 3, thick solid line) shows strong energy dependence below $E=0.1$ eV, nitrogen molecule essentially presents no energy dependence at the same energy range [17]. It is opportune to recall that such behavior may indicate the existence of a nearly zero-energy virtual state, i.e., a quasi-bound state of the e^+-C_2H_2 compound system. Once SMC deals with square integrable variational basis sets [20], we can diagonalize the scattering Hamiltonian, thus obtaining a pseudospectrum and pseudoeigenstates that may in turn be used as trial wave functions [26]. In carrying out such diagonalization, we found that the three lowest-lying vectors have eigenvalues ranging from 2×10^{-3} to 6×10^{-2} hartree. We

TABLE I. Polarizabilities (a_0^3) of C_2H_2 molecule.

Result	$\alpha_\parallel$	$\alpha_\perp$	$\alpha_{average}$	$\Delta\alpha$
Experiment [25]	30.73	18.83	22.8	11.9
Present	31.03	19.22	23.16	11.81
Ref. [24]	28.86			

then performed a calculation using the pseudoeigenvectors as trial functions, but *removing* the three lowest-lying states. This resulted in a smaller (and roughly constant) ICS in the $E\to0$ limit (see Fig. 3, dashed line).

We also estimated the scattering length α by extrapolating our data according to the definition [27]

$$\alpha=-\lim_{k\to0}\frac{1}{k}\tan[\delta_0(k)], \tag{7}$$

where k is the positron momentum and δ_0 is the *s*-wave phase shift, obtaining $\alpha=-229a_0$. This corresponds to a virtual state at $\kappa=2.6\times10^{-4}$ eV. This result is considerably larger (absolute value) than scattering lengths estimated for C_2H_4 and atomic targets [6]. We recall that a true zero-energy resonance is a purely mathematical result, in which $\alpha\to-\infty$ as $E\to0$ [27]. In actual physical systems, one finds low-lying virtual states with slightly positive energies and large (though finite) negative scattering lengths. We also point out that our ICS is not far from the unitary limit of the *s*-wave elastic cross section, $\sigma\simeq4\pi k^{-2}$ (see Fig. 3), indicating that our description of e^+-target interaction approaches the maximum scattering theoretical limit.

Further evidence of the existence of an e^+-acetylene virtual state was provided by *s*-wave phase shifts δ_0. According to Levinson's theorem [27], an ideal zero-energy resonance should behave like $\delta_0(E\to0)=\pi/2$. In actual systems, δ_0 will always go to zero as $E\to0$, though it is expected to get closer to $\pi/2$ and fall more abruptly as the interaction potential becomes more attractive, i.e., as the virtual state energy approaches zero (see Ref. [27], pp. 86–91). In Fig. 4 our calculated *s*-wave phase shift (solid line) is compared with the result obtained by removing the three lowest-lying vectors (dashed line). We also show results for a model box potential, defined by the range $a=10a_0$ and by the dimen-

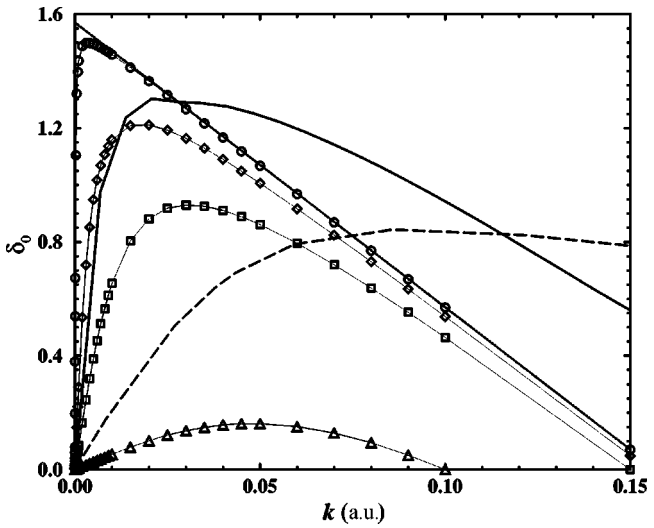

FIG. 4. *s*-wave phase shifts for e^+-C_2H_2 collisions. Solid line: present result; dashed line: present result removing the three lowest-lying pseudoeigenstates of the scattering Hamiltonian. Further results were obtained for scattering by a model box potential (see text). Triangles: $\kappa a=0.75$; squares: $\kappa a=1.00$; diamonds: $\kappa a=1.55$; circles: $\kappa a=1.57$; dotted line: $\kappa a=\pi/2$ (zero-energy resonance).

sionless parameter κa, where $\kappa=\sqrt{k^2+U_0}$ [27]. At low impact energies ($ka \ll 1$), the potential strength U_0 will eventually bear a virtual state,

$$\kappa a \to \frac{\pi}{2} \Rightarrow \lim_{k\to 0} \delta_0(k) = \frac{\pi}{2}, \tag{8}$$

where δ_0 is the *s*-wave phase shift. It may be noticed in Fig. 4 that our calculated δ_0 resembles the box potential result for $\kappa a=1.55$, while the result obtained without the lowest-lying states is intermediate between $\kappa a=0.75$ and $\kappa a=1.00$. Even though square potential results quantitatively depend on the chosen range *a*, Fig. 4 indicates that the e^+-C_2H_2 potential bears a virtual state.

C. Possibility of bound-state formation

In order to check the convergence of our variational trial space at very low energies, we augmented the Cartesian Gaussian set described in Ref. [17] by completely uncontracting the primitive basis functions (that is, by setting all contraction coefficients equal to unit). As a result, the number of configurations belonging to the global A_g symmetry increased from 6053 to 10376. We then performed a new round of scattering calculations with such larger configuration space (A_g symmetry only). In view of the very high computational effort, only a few selected collision energies were addressed. The result is presented in Fig. 3 (diamonds) and it is clear that our previous calculation was well converged at room temperature (10^{-2} eV). Below 10^{-3} eV, the augmented configuration space brought noticeable improvement, lying even closer to the unitary-limit cross section. We mention in passing that the scattering length was enhanced to $\alpha=-605a_0$, corresponding to a virtual state with $\kappa=3.7\times10^{-5}$ eV.

Before making any considerations about the possibility of finding a bound state by further improving the configuration space, one should keep track of the approximations made so far: fixed nuclei and target described at the restricted Hartree-Fock (HF) level. If description of correlation effects in the e^+-acetylene system was improved (by either augmenting the Gaussian basis set or by taking double excitations into account), an unphysical bound state would eventually be created due to overcorrelation [that is, due to the unbalance between a highly polarized $(N+1)$-particle system and a HF target]. Such a spurious bound state would become virtual (slightly positive energy) again by improving target description. Needless to say that thoroughly correlating both the target and the compound e^+-C_2H_2 system within the SMC framework is not at all feasible in view of computational limitations. Unfortunately, formation of a physical bound state cannot be predicted based on present results. We observe, however, that the existence of either a shallow bound state or of a low-lying virtual state is expected to affect the annihilation rate in a similar fashion. In both cases, the elastic cross section would behave like $\sigma(k\to 0)\to 4\pi/\alpha^2$, the scattering length being negative for a virtual state or positive for a bound state [27]. Since fixed-nuclei annihilation parameters ($Z_{\rm eff}$) and elastic cross sections should have the same energy dependence [28], $\propto(k^2+\kappa^2)^{-1}$, the room-temperature annihilation rate is not expected to be dramatically affected by formation of a shallow bound state. Room-temperature $Z_{\rm eff}$ measurements are usually averaged over the Maxwellian distribution of positron momenta, thus being insensitive to small shifts of either bound or virtual states, as far as they lie very close to $E=0$ or, put in other words, as far as $|\kappa^2/2| \ll 0.0257$ eV. This situation corresponds to the largest contribution to $Z_{\rm eff}$ within the fixed-nuclei approximation (deeper bound states would yield smaller cross sections and smaller annihilation parameters).

Finally, we point out that a different picture would be found if nuclear motion was taken into account. In such a case, energy could be transferred from the positron to the nuclei thus forming metastable vibrationally excited bound states (vibrational Feshbach resonances) [6]. Such states are expected to remarkably increase the (Maxwellian averaged) annihilation rates, depending on the density of the vibrational spectrum of the e^+-target system. The energy dependence of acetylene's $Z_{\rm eff}$ was recently measured [29] and it presented a sharp peak around 0.1 eV, corresponding to the lowest-lying Feshbach resonance. However, it was found that $Z_{\rm eff}=1400$ on the resonant peak, which is rather small as compared to the (Maxwellian averaged) room-temperature value ($Z_{\rm eff}=3160$ [16]). As a result, the Feshbach resonance mechanism seems not to account for acetylene's room-temperature annihilation rate, especially if we recall that the Mawellian profile is very sharp, being essentially zero around 0.1 eV (for $T=300$ K). This indicates that virtual state formation would be the predominant annihilation mechanism. Moreover, if some average over the molecular

geometry was performed, its effect would be essentially shifting the virtual state (or bound state) energy thus having little influence on the room-temperature annihilation rate.

D. Annihilation

No similar evidence of an e^+-nitrogen virtual state was found [17]. In fact, as $E \to 0$ the elastic cross section remains essentially constant, and the *s*-wave phase shift smoothly goes to zero. Moreover, the experimental room temperature Z_{eff} of C_2H_2 exceeds that of N_2 by 100 times, in agreement with the previously pointed out connection between virtual states and annihilation rates [2,7]. Our calculated room temperature Z_{eff} for C_2H_2 and N_2 are 145.1 and 9.34, respectively, being underestimated with respect to experimental data [19]. Despite this error, Z_{eff} curves for these molecules present strikingly different qualitative behaviors [17]. Below 0.1 eV, nitrogen result for Z_{eff} is quite flat. On the other hand, large derivatives are found for acetylene, though significant change is introduced by removing the three lowest-lying states, as already observed for ICS (see Fig. 3). Hence, these qualitative features also suggest that formation of an e^+-C_2H_2 virtual state should enhance annihilation rates. As a matter of fact, Gribakin [29] has derived the following expression for Z_{eff} in the presence of a virtual state:

$$Z_{\text{eff}} = Z_{\text{eff}}^{(0)} \frac{\kappa^2}{k^2 + \kappa^2}, \tag{9}$$

where $Z_{\text{eff}}^{(0)}$ is the annihilation parameter at zero positron energy. This relation is valid at low impact energies ($E \to 0$) and neglects nuclear motion, thus being comparable with the present theory. As discussed elsewhere [19], the SMC framework is based on Cartesian Gaussian basis sets, which are unable to accurately describe the wave function cusp. This limitation is not important as far as the positron is scattered (therefore not affecting calculated cross sections), but it becomes severe for Z_{eff} calculations due to the Dirac's delta function in Eq. (4). As a result, our method is expected to accurately describe the energy dependence of the annihilation parameter, even though it would underestimate the factor $Z_{\text{eff}}^{(0)}$ in Eq. (9), which accounts for short-ranged interactions. Even though this puzzles direct comparison between present Z_{eff} calculations with Eq. (9), we may take advantage of previously calculated virtual state energies and of Eq. (9) to plot

$$\log Z_{\text{eff}} = \log Z_{\text{eff}}^{(0)} + \log[\kappa^2/(\kappa^2 + k^2)]. \tag{10}$$

The results are presented in Fig. 5. For both basis sets, we carried out a linear regression of our data ($y = ax + b$) by using the four points corresponding to the lowest energies, namely 10^{-4}, 10^{-3}, 10^{-2}, and 0.0257 eV [Eqs. (9) and (10) are expected to be accurate in the $E \to 0$ limit]. We thus obtained the slopes $a = (0.995 \pm 0.003)$ for the basis set of Ref. [17] and $a = (0.989 \pm 0.003)$ for the augmented basis set. These results agree very well with the expected slope $a = 1$ [see Eq. (10)], indicating that our calculated Z_{eff} indeed present the energy dependence related to the existence of a virtual state.

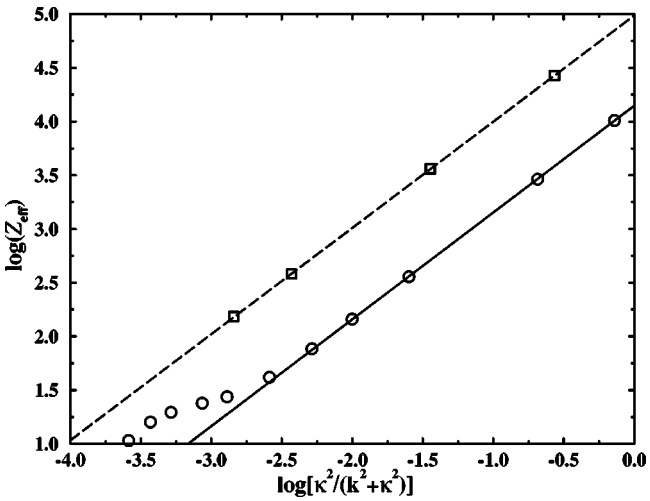

FIG. 5. Plot of $\log(Z_{\text{eff}})$ vs $\log[\kappa^2/(k^2+\kappa^2)]$ (see text). Circles: present result obtained with the uncontracted basis set of Ref. [17]; solid line: linear regression of our data (basis set of Ref. [17]); squares: present result obtained with the uncontracted (augmented) basis set; dashed line: linear regression of our data (augmented basis set).

V. CONCLUSIONS

In conclusion, our calculated DCS and ICS reasonably agree with available experimental data. We also provided evidence of the existence of a low-lying e^+-acetylene virtual state. Our description of the interaction potential is variational, thus depending on trial basis sets. As a result, the energy of the virtual state, as well as the behavior of cross sections and phase shifts, may change as the basis set is improved. Nevertheless, the existence of either a shallow bound state or a low-lying virtual state would be irrespective, as long as (Maxwellian averaged) room-temperature annihilation rates are concerned. It should be also pointed out that vibrational Feshbach resonances are not expected to play a crucial role in room-temperature e^+-acetylene scattering [28]. As a result, the annihilation process would be essentially determined by the fixed-nuclei virtual state formation (even some geometry average would not dramatically affect the annihilation rate because it would only slightly shift the virtual state energy). Our cross sections are close to the *s*-wave unitary limit thus indicating a thorough description of correlation effects, which in turn seem to be attractive enough to bear a virtual state. The SMC framework, based on trial Gaussian basis sets, is not able to accurately describe the wave function cusp. As a consequence, our Z_{eff} calculations are underestimated with respect to experience [19]. Nonetheless, our results show the expected energy dependence, therefore supporting the existence of a virtual state. Once the e^+-acetylene annihilation process seems to be understandable by means of (fixed-nuclei) virtual state forma-

tion, a sharp prediction of the experimental room-temperature annihilation rate would depend on improving the description of short-ranged interactions (that is, of the wave function cusp). Strategies for such a purpose are being currently discussed in our group.

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