Positronium formation from He, Be, C, O, and Ne by the impact of high-energy positrons

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Positronium formation from He, Be, C, O, and Ne by energetic positrons has been studied using an approximation which is complete through all second-order terms in collisional potentials. We have calculated differential and total positronium-formation cross sections for a wide range of energies. We obtain clear evidence of residual structure near the Thomas angle in the keV range of energies due to the destructive interference of second-order amplitudes. At a fixed energy this structure gradually disappears as the target charge increases and for a fixed target this structure becomes more prominent with the increase of energy. The total cross section for capture by positrons ($\sigma_{\rm Ps}$) in the present method differs from the corresponding cross sections for capture by protons ($\sigma_{\rm H}$) at least by an order of magnitude at the same velocity. Our cross sections are qualitatively different from the first-order Brinkman-Kramer results. For example, the ratio $\sigma_{\rm Ps}/\sigma_{\rm H}$ decreases with the increase of energy in the present method whereas in the Brinkman-Kramer approximation this ratio increases slightly. A number of possible experimental tests are discussed.

I. INTRODUCTION

Positron-impact rearrangement collisions are now emerging as a useful way to gain new insight into electron capture in both theoretical and experimental atomic physics. Total cross sections for electron capture by positrons from hydrogen atoms[1] are predicted to be larger by an order of magnitude than for electron capture by protons at the same velocity in proton-hydrogen collisions. At present there is no experimental test in atomic hydrogen because it is difficult experimentally to use the hydrogen atom as the target. However experiments[2–4] are now being done in atomic or molecular targets containing more than one electron, e.g., He, which are easier to use experimentally. In a very recent measurement in helium Fromme *et al.*[4] observed that the ratio $\sigma_{\rm Ps}/\sigma_{\rm H}$ for $v=3.9$ is about 25, which is qualitatively consistent with our earlier prediction[1] for atomic hydrogen. Hence to compare theory and experiments it is worthwhile[5] to apply our earlier method[6] for positronium (Ps) formation to targets other than atomic hydrogen. In this paper we present calculations for various atomic targets which are experimentally accessible.

It is not yet clear whether the capture mechanism in positron-atom scattering is a two-step process, as it is for an ion-atom collision, or an even higher-order process. The angular distributions of these cross sections can provide information about the nature of this capture mechanism. In ion-atom collisions the observation of the Thomas peak[7] in the angular distribution of the cross sections[8–10] confirmed the prediction[7,11,12] that capture is a two-step process. For positronium formation it has been predicted that two second-order Thomas-like mechanisms interfere destructively[13,1] in $1s$-$1s$ capture eliminating the Thomas peak in the differential cross sections. However, the nature of the residual structure near the Thomas angle due to the destructive interference of second-order amplitudes is not yet well understood.

Relatively few attempts have been made to calculate positronium-formation cross sections from nonhydrogenic atoms in the intermediate- and high-energy region. Drachman *et al.*[14] developed a method in the two-state coupled static approximation which may be applicable to study a system such as $e^{+}+{\rm He}$ at high velocities, but they gave results for $e^{+}+{\rm H}$ only at low and intermediate energies. A classical trajectory Monte Carlo calculation has been done for $e^{+}+H$ by Ohsaki *et al.*[15] and first Born calculations have been reported, again for $e^{+}+H$ by Ma *et al.*[16] Also Mandal *et al.*[17] studied the positronium formation in hydrogen including the distortion potential to all orders but they neglected some second-order terms such as $V_{Te}V_{Pe}$ and $V_{PT}V_{Pe}$ which are needed in the high-energy region. In a review article Ghosh *et al.*[18] discussed the low-energy positronium formation and some elastic scattering for $e^{+}+{\rm He}$ system. Shakeshaft and Wadehra[13] presented an insightful calculation that can be applied for targets of high nuclear charges. Their distorted-wave Born calculation treated the second-order terms such as $V_{Te}G_0V_{Pe}$ and $V_{PT}G_0V_{Pe}$ where V_{PT}, V_{Te} and V_{Pe} are the positron-target, target-electron, and positron-electron interactions and G_0 is the free-particle Green's function. They presented some results for $e^{+}+{\rm H}$ system up to 200 eV, and their method is applicable to systems such as $e^{+}+{\rm He}$ and targets of higher nuclear charge. However, they used the plane-wave intermediate states which are not always adequate to describe the angular distribution near the Thomas peak as pointed out by Briggs *et al.*[19] who advocate Coulomb distorted intermediate states, such as we use in this paper. Also Shakeshaft and Wadehra[13] omitted some of the second Born contributions. We include all second Born contributions in our calculation. In the present theoretical investigation we consider the differential and total cross sections for the reactions $e^+ + A(1s) = \mathrm{Ps}(1s) + A^+$, where A represents the atomic targets He, Be, C, O, and Ne. We have used the earlier developments of Deb *et al.*[6,1] with necessary changes in reduced mass, effective target charge, etc., for the present investigation. In the next section we briefly describe our method of calculation. Atomic units are used throughout the work and all the notations used here are consistent with our earlier works.[1,6]

II. THEORY

The basic transition matrix element is given by

$$T = \langle \psi_f \mid \bar{V}_f (1 + G^+ \bar{V}_i) \mid \psi_i \rangle \ , \tag{1}$$

where ψ_i and ψ_f are initial target state and final positronium state wave functions. G^+ is the total Green's function, $\bar{V}_i$ and $\bar{V}_f$ are the interactions in initial and final channels, respectively. It is to be noted here that in the present calculation we include the "internuclear" potential $V_n = Z_T/R$ which is generally excluded for electron capture by heavy particles. Here Z_T is the effective target charge and R is the distance between positron and the target nucleus. In order to evaluate amplitudes in our method, it is convenient to express the exact T matrix as

$$T = T_1 + T_2 - T_3 \tag{2}$$

with

$$T_1 = \langle \psi_f \mid (Z_T/R - Z_T/r)[1 + G^+(Z_T/R)] \mid \psi_i \rangle \ , \tag{3a}$$

$$T_2 = \langle \psi_f \mid (Z_T/R - Z_T/r)[1 + G^+(-1/\rho)] \mid \psi_i \rangle \ , \tag{3b}$$

$$T_3 = \langle \psi_f \mid (Z_T/R - Z_T/r) \mid \psi_i \rangle \ , \tag{3c}$$

where $\mathbf{r}$ and $\boldsymbol{\rho}$ are the position vectors of the active atomic electron with respect to the target nucleus and the positron, respectively.

In our calculation we include all terms second order in the potentials V_i, V_f, and V_n where $V_i = -1/\rho$, $V_f = -Z_T/r$, and $V_n = Z_T/R$. In principle with the three potentials V_i, V_f, and V_n there are nine possible second-order terms: $V_iGV_i, V_iGV_f, V_iGV_n$; $V_fGV_f, V_fGV_i, V_fGV_n$; $V_nGV_n, V_nGV_i, V_nGV_f$. However, since $\langle \psi_i \mid V_i G = \langle \psi_i \mid$ and $GV_f \mid \psi_f \rangle = \mid \psi_f \rangle$, five of these terms reduce to first-order terms so that V_nGV_i, V_fGV_i, V_nGV_n, and V_fGV_n are the only four second-order terms. These are the four second-order terms in Eqs. (3a) and (3b) in the exact expression for T. The V_nGV_i term gives a second-order peak in ion-atom scattering. The V_fGV_i term gives a second-order singularity at 60° in ion-atom scattering. It is these terms whose second-order singularities cancel at 45° for 1s-1s capture by positrons as first illustrated by Shakeshaft and Wadehra.[13] The remaining second-order terms, V_nGV_n and V_fGV_n, have no singular contributions like the Thomas term. In ion-atom scattering they are generally ignored since by Wick's theorem they are quite small, namely of the order of (m/M_p) where m (M_p) is an electron (projectile) mass. When $M_p = m$, as is the case for positron impact, these terms cannot be ignored. All four terms are illustrated in Fig. 1. The last two terms include effects of the positron-nuclear Coulomb interaction on ψ_i giving rise to Coulomb distortions on ψ_i. Hence they have been referred to as second-order distortion terms. In atomic hydrogen it is these second-order distortion terms that prevent the cross section from going to zero at 45° in a second-order calculation.[1]

In the calculations presented here the matrix elements T_1, T_2, and T_3 are evaluated following the method of Deb *et al.*[6] developed for $e^+ + H$. Specifically the full Green's function G^+ in T_1 is approximated by a Coulomb Green's function by ignoring the $-1/\rho$ potential in G^+. In T_2, which contains the two singular second-order Thomas-like terms, $Z_T(1/R - 1/r)$ is ignored in G^+. Thus the intermediate states in T_1 propagate in the Coulomb field of target and those in T_2 propagate in the Coulomb field of positron. Since we approximate the initial-state wave function of helium as a hydrogenic wave function the expressions for the matrix elements are quite similar except for changes in parameters involving reduced mass, effective target charge, $Z_T = 1.69$ and binding energy $\varepsilon_{1s} = 24.6$ eV. The matrix elements then can be evaluated as

$$T_1 = 16\pi^2 C \int_0^\infty \left[\left[\frac{\partial}{\partial \lambda} \frac{\partial}{\partial \beta_1} \lim_{\varepsilon \to 0} X(G,H) \right] - \left[\lim_{\varepsilon \to 0} \frac{\partial}{\partial \varepsilon} \frac{\partial}{\partial \beta_1} X(G,H) \right] \right] dv \ , \tag{4}$$

$$T_2 = \sum_{k=1}^{3} \sum_{j=0,x,y,z,x\ln G} \int_0^\infty dp\, p^2 f'(p) a'_{kj} 2\pi \mathcal{J}'_{kj} \ , \tag{5}$$

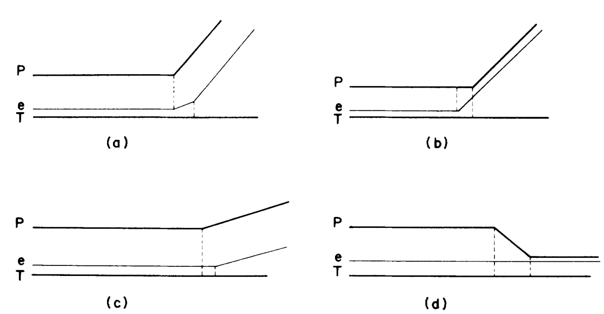

FIG. 1. Diagrams for second-order contributions for capture by positrons. (a) represents the singular Thomas term, (b) represents a term which is singular at 60° for heavy projectiles, (c) and (d) represent the Coulomb distortion terms. For capture by positrons (a) and (b) are singular at 45° and these singularities cancel for 1s-1s capture (cf. Refs. 1 and 13).

$$T_3 = 8\pi Z_T (Z_T\beta_1)^{3/2} \frac{\partial}{\partial\lambda}\frac{\partial}{\partial\beta} L(U_1,V_1,W_1) - \frac{32\pi^2 (Z_T\beta_1)^{5/2}}{[(\mathbf{K}_i-\mathbf{K}_f/2)^2+\beta_1^2]^2[(\mathbf{K}_i-\mathbf{K}_f)^2+\lambda^2]} , \quad (6)$$

where all the parameters in Eqs. (4)–(6) are listed in the work of Deb *et al.*[6] We evaluate the one-dimensional integrals in Eqs. (4) and (5) following the numerical technique of Sil and McGuire.[20]

III. RESULTS AND DISCUSSION

We have calculated total and differential 1*s*-1*s* cross sections for Ps formation in various atomic system for wide range of energies. The wave functions for the *k* shell of the various targets considered here are taken to be hydrogenic and the effective target charge are taken in accord with variational calculations for the ground state of two electron ions, namely $Z_T = Z_N - 5/16$, where Z_N is the atomic number. In Fig. 2 we plot the differential cross sections for Ps formation in He as a function of scattering angle for energies from 500 to 100 keV. The solid line is our result (DMS) and dashed line is the Brinkman-Kramer (BK) result. At the higher energies some structure is evident near 45°. This structure is due to an interference between T_1 and T_2 in Eq. (2). As demonstrated earlier,[1] T_2 changes sign at 45° when the two second-order singular terms cancel. The two second-order distortion terms in T_1 are smoothly varying. Consequently at $\theta < 45°$ there is a constructive interference between T_1 and T_2 and for $\theta \geq 45°$ the interference is destructive. This interference structure of the cross sections is becoming more prominent as the energy increases. It is significant to note that the structure of the corresponding Thomas peak for electron capture by protons[21] is much larger at comparable collision velocities, v. The difference is that in the present case we are getting a residual structure due to the destructive interference of second-order amplitudes, whereas McGuire *et al.*[21] obtain the full Thomas peak.

Figure 3 shows how the differential cross sections at a fixed energy, 10 keV, varies with the increase of target charge. The interference structure disappears as the target charge Z_T increases or v/Z_T decreases. Another interesting observation is that for He the BK results is somewhat larger than DMS up to about 45°, but at large angles the BK result is several orders of magnitude smaller than our DMS result. However, for $e^+ + \mathrm{Ne}$ our DMS result is nearly twice as big as those of BK in the extreme forward angle. Even a relatively inaccurate experiment would distinguish between DMS and BK at large angles. As Z_T increases DMS becomes larger than BK at forward as well as backward angles. For proton impact dividing the cross section by a factor of 3–10 gives fairly reliable total cross sections as a function of Z_T and v for protons and in this way BK predictions are often used[22] to ana-

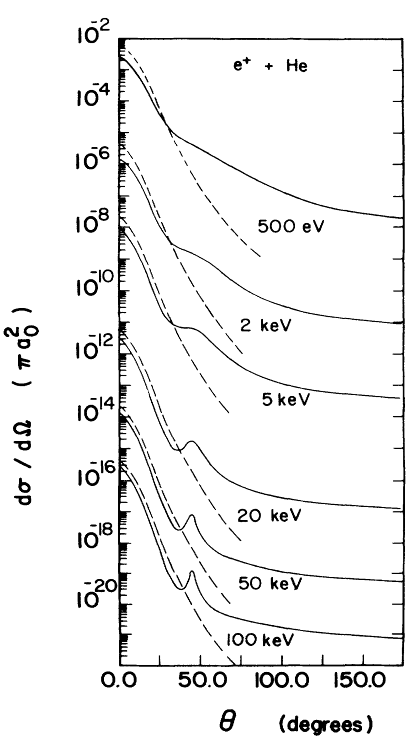

FIG. 2. Differential cross sections as a function of scattering angle, θ, for electron capture by positrons in units of πa_0^2 at several energies for $e^+ + \mathrm{He}$. The solid line is the present result the and dashed line is the Brinkman-Kramer result.

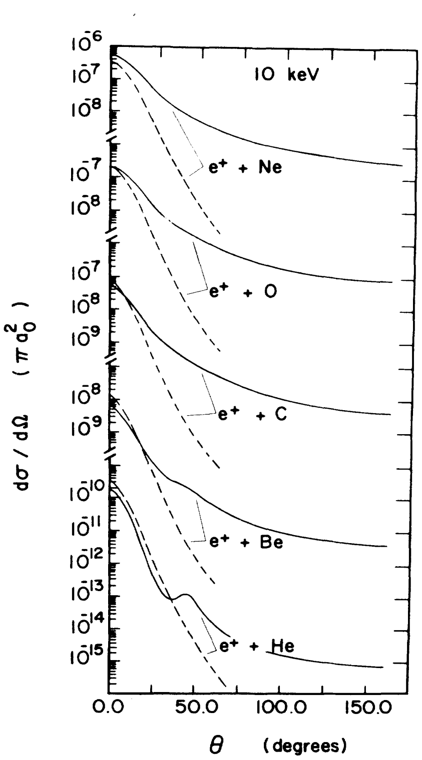

FIG. 3. Differential cross sections in units of πa_0^2 for electron capture by positrons from various targets at a fixed energy 10 keV.

lyze the capture data. If DMS is correct then BK total cross section may not be as useful for positron impact as for proton impact.

Various first-order theories,[16–18] including the projectile nuclear potential Z_T/R, have predicted a dip in the differential cross section near 45°. This dip is due to the cancellation between Z_T/R and Z_T/r [cf. Eq. (3)] which happens to occur near 45°. We note that this dip is also present if our second-order Coulomb distortion terms are ignored.[1] Since near 45° the cancellation of Thomas singularities occurs and various theories seem to differ most, experimental observation of the differential cross section about 45° would be helpful.

The Thomas-type singularities are mass dependent.[23] Normally there are two peaks in the differential cross sections corresponding to two second-order singular terms. For protons on heavy targets one peak[11] is at the very forward angle $\theta_T=(1/M_p)\sin(\pi/3)$, where M_p is the mass of the projectile and the other[8] peak is at $\theta=\pi/3$. The first amplitude corresponding to Fig. 1(a), corresponds to the electron scattering from the projectile and then from the target nucleus. The second singular amplitude corresponds to the projectile scattering from the electron and then from the nucleus. As the mass of the projectile M_p decreases somewhat $\theta_T=(1/M_p)\sin 60°$ increases somewhat. As M_p approaches the mass of the captured electron both peak moves toward 45°. Since for 1s-1s capture the signs of the amplitudes for these two singularities are opposite,[1,13] they cancel for capture by positrons and the peak disappears. If the differential cross section could be observed for relativistic positrons, then as the mass of the positron increased two peaks would develop and move, as the mass increased, in opposite directions away from 45°.

Figure 4 shows a comparison of our results with experimental data[3,4] in helium. Below 170 eV both our DMS result and the BK result are much too high. This is not surprising since both theories are based on an expansion in Z_T/v which is not small at low energies. Furthermore, our calculation may not give correct cross sections at low energies due to our use of the peaking approximation valid at high velocities, $v \gg 1$. Above 170 eV our results are consistent with observation.[3,4] In this experimentally difficult region the uncertainties in observed results are large. However, we do note that a rough fit between $E=120$ and 200 eV to the data[3,4] varies as E^{-1}, while the theory varies as E^{-5}. There is general agreement among theorists that at asymptotically high energies the 1s-1s cross section varies as E^{-6}. In our opinion 250 eV is a high energy for helium, i.e., $v/Z_T=2.5>1$, but not quite asymptotic. Here v is the projectile velocity in atomic units. And cross sections for electron capture by protons in helium do fall[24] off much faster than E^{-1} at these velocities. If further observation confirms an E^{-1} dependence, then this result is likely to lead through to new insight about capture by positrons at high velocity.

In Fig. 5 we plot the ratio σ_{Ps}/σ_H of total cross sections for Ps formation in $e^+ + \text{He}$ collision to the corresponding results of H-atom formation in $p+\text{He}$ collision as a function of v/Z_T. Both our DMS result and BK result shows that Ps formation cross sections are higher than H-atom formation cross sections at least by an order of magnitude. Physically $\sigma_{Ps}>\sigma_H$ because the positron slows down during the collision to share its kinetic energy with the electron to conserve overall energy. The proton does not slow down significantly since it is relatively massive. Because the capture cross section increases rapidly as v decreases, σ_{Ps} is larger than σ_H. We also note that the geometric cross section[16] for Ps is four times larger than for H. For DMS the ratio σ_{Ps}/σ_H falls rapidly with v/Z_T up to about 15 and then continues to fall very slowly. The corresponding BK ratio, however, rises slowly with increasing energy. These results both indicate that capture cross sections may not scale with projectile mass in a simple way, i.e., independent of projectile velocity as suggested by the results of Ma *et al.*[16] who considered $e^+ + H$ and $\mu^+ + (\mu^-, p)$. Since DMS and BK give different energy dependences of the ratio σ_{Ps}/σ_H, observation of this energy dependence would be informative.

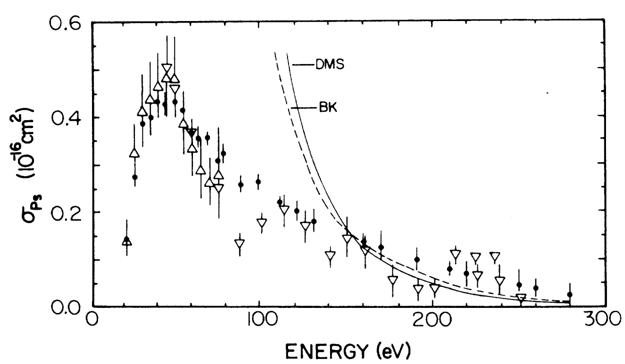

FIG. 4. Total cross sections for $e^+ + \text{He}$ at energies up to 300 eV. Theoretical results: DMS is our present result and BK is the Brinkman-Kramer results. Experimental data: ●, Fromme *et al.*; ▽, Diana *et al.*; △, Fornari *et al.*

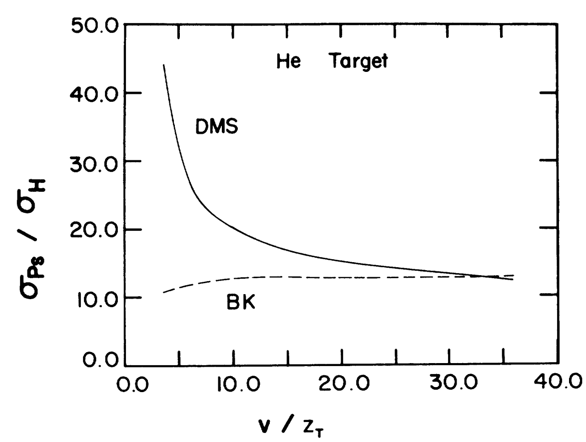

FIG. 5. Ratio of the Ps formation cross section in $e^+ + \text{He}$ to the H atom formation cross sections in $p+\text{He}$ collisions. DMS and BK are our present and Brinkman-Kramer results, respectively.

TABLE I. Total Ps formations in units of πa_0^2 at 10 keV from various targets. DMS is the present result and BK is the Brinkman-Kramer result. The negative integers within the square brackets are the powers of 10 by which the corresponding numbers are to be multiplied.

	DMS	BK
He	2.144[−11]	5.607[−11]
Be	1.529[−9]	2.249[−9]
C	1.762[−8]	6.975[−9]
O	8.846[−8]	3.991[−8]
Ne	2.845[−7]	7.363[−8]

In Table I we tabulate the total positronium formation cross sections in the DMS and BK approximations at 10 keV for targets between $Z=2$ and 10. The total cross sections increases as the target charge increases. The rate of this increase diminishes with the increase of target charge. For example our DMS result for Be is nearly 100 times than that of He whereas DMS for Ne is nearly ten times than that of C and nearly three times than that of O. The corresponding BK results also increases with target charge but the rates of increase are smaller than those of present results. In Table II we present total cross sections for positronium formation from He using DMS and BK methods as well as corresponding results for H-formation of Sil and McGuire (SPSM) (Ref. 21) at several energies.

Electron capture by positrons is not so well understood as electron capture by protons. In part this is because capture by positron has not been studied as extensively as capture by protons either experimentally or theoretically. It is also true that capture by positron is simply more complicated due to the cancellation of the Thomas-type singularities. In studies of positronium formation, particularly differential studies, one may "look under" the Thomas peak, i.e., consider directly the residue left after cancellation of leading-order Thomas terms. While the leading second-order Thomas amplitudes have been understood in terms of intermediate states of ionization,[25] our amplitudes appear to be more complicated, since the singular second-order terms cancel. We note, for example, that our T_2 capture amplitude is equal to the integral of a difference of amplitudes for ionization by electrons and positrons weighted by the final-state momentum wave function, i.e.,

$$T_{2_{\text{cap}}}^{e^+} = \int d\mathbf{p}(T_{\text{ion}}^{e^+} - T_{\text{ion}}^{e^-})\phi_f(\mathbf{p}) .$$

Knowledge of the corresponding intermediate states, which may contain significant off-shell contribution,[26] may give insight into the physical origins of the difference of ionization by positrons and electrons. It might also be interesting to reconsider the interpretation of the Thomas peak as a momentum transfer resonance[27] when destructive interference occurs, i.e., for capture by positrons. Again in atoms capture by positrons requires a deeper physical understanding than capture by protons. It is possible that capture from positronium by positrons (or electrons) may require even deeper understanding, and it is amusing to speculate[28] about possible CPT violations that might be discovered by studying differences in capture from positronium by electrons and positrons.

Our calculations, while complete through second Born, still contain large uncertainties especially at the lower velocities considered here. It is uncertain how much error is introduced by the high-velocity peaking approximation we employ. Since our codes are numerically stable at lower velocities for positron capture than for proton capture, we have presented results in this paper at velocities which may be somewhat low for the peaking approximation to be valid. We ignore some third-order terms which are difficult to evaluate. It is possible that even at higher velocities third Born terms are significant. And we have ignored capture to excited final states. For odd $\Delta\ell$ transition (e.g., $1s$-$2p$), the interference of the two Thomas amplitudes is constructive, and would make some contribution to the differential cross section near 45°. These uncertainties could be as large as a factor of 2 or so. Consequently the spirit of this paper is to focus on general qualitative effects larger than a factor of 2 and to point to observable effects that may lead to a clearer understanding of the relatively difficult problem of electron capture by positrons.

IV. SUMMARY

We have presented calculation of cross section for positronium formation from various atomic targets at high velocities. Our DMS calculation includes all four possible

TABLE II. Total Ps formation cross sections from He atom in units of πa_0^2. DMS is the present result and BK is the Brinkman-Kramer result. SPSM is the electron capture cross sections in units of πa_0^2 in proton-helium collision (Ref. 21). The negative integers are the powers of 10 by which the corresponding numbers are to be multiplied. Z_T is defined in the text.

Positron Energy (eV)	v/Z_T	DMS	BK	SPSM
300	2.78	7.936[−3]	1.233[−2]	1.312[−4]
500	3.59	5.633[−4]	1.134[−3]	1.280[−5]
1000	5.07	1.265[−5]	3.146[−5]	4.115[−7]
2000	7.17	2.484[−7]	6.722[−7]	1.074[−8]
5000	11.37	1.238[−9]	3.354[−9]	6.511[−11]
10000	16.05	2.144[−11]	5.607[−11]	1.309[−12]

second-order terms. We include the "internuclear" potential generally excluded in electron capture by heavy particles which contributes significantly to our result for capture by positrons. Several experimental tests are suggested including studies of differential cross section, especially near 45°, energy dependence of the total cross sections above 150 eV, and energy dependence of the ratios of total cross section for capture by positrons and protons at the same velocity.

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