Low-energy positron collisions with H_2 and N_2 molecules by using a parameter-free positron-correlation-polarization potential

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We employ a parameter-free positron-correlation-polarization (PCOP) potential to calculate total (rotationally summed) cross sections for the positron-H_2 (N_2) collisions below the positronium formation threshold energy. A laboratory frame close-coupling technique, retaining six rotational states ($j = 0, 2, 4, 6, 8, 10$), has been used. It is found that the PCOP model compares reasonably well with measured values. Results on rotationally elastic and inelastic cross sections are also reported. We also make a comparison between PCOP and electron-correlation-polarization models for all the cross sections reported here.

One of the major problems in low-energy positron collisions with atoms and molecules is the inclusion of polarization effects nonempirically.[1-5] It is still an unsolved problem and any simplified version of such charge correlation effects is worth investigating theoretically. In this paper, we have reported total cross sections for the e^+-H_2 and N_2 systems by employing a simple parameter-free polarization potential,[6-8] which is derived analytically in terms of target charge density. In brief, the new potential, known as the positron-correlation-polarization (PCOP) potential,[6-8] is based on the correlation energy of a positron in a homogeneous electron gas at short distances and the correct asymptotic form ($-[\alpha_0 + \alpha_2 P_2(\cos\theta)]/2r^4$ where α_0 and α_2 are, respectively, the spherical and nonspherical polarizabilities of the molecule) at larger distances.

The PCOP model was tested successfully for atomic and molecular targets.[6-8] Here our goal is to employ the PCOP potential for H_2 and N_2 molecules for which a large number of theoretical and experimental studies are available (see a recent review by Armour[9] for references prior to 1988). More recently Mukherjee, Sur, and Ghosh[10] have summarized the e^+-N_2 work. Earlier, Ghosh, Sil and Mandal[11] have reviewed theory on the positron-molecule collisions. The issue of polarization potential has been discussed by Morrison and co-workers for e^+-H_2 (Morrison, Gibson, and Austin[1]) and e^+-N_2 (Elza *et al.*[2]) systems. It is now quite obvious after several theoretical studies[1-5] that it is not appropriate to employ electron polarization potential for the case of positron scattering. In a more sophisticated R-matrix-type approach,[12-15] the problem of including such charge correlation and polarization effects exactly still remains there. Moreover, for practical purposes, it is always worth looking for simplified models for polarization interaction in positron scattering problems. Armour and co-workers (see Armour, Baker, and Plummer[16] and

references therein) have studied the e^+-H_2 collision using the Kohn variational method.

Certainly, the polarization and correlation effects are very important in low-energy e^+-molecule collisions. Without the inclusion of such effects, even the R-matrix calculation[12] for e^+-H_2 and e^+-N_2 systems are very poor when compared with experimental data. The corresponding differential and other low-energy parameters (such as scattering length and annihilation cross section) are very sensitive to polarization of the target. In addition, the inelastic processes (for example, rotational and vibrational excitation) are also quite sensitive to the approximations involved in the calculation of polarization potential. The PCOP model[6-8] is being applied here for the first time to these H_2 and N_2 molecules for rotationally elastic, inelastic, and summed cross sections.

The theory and numerical procedure of the present calculations are exactly the same as described in Mukherjee, Sur, and Ghosh.[10] The description of the PCOP potential is given by Jain.[6-8] Here we give only a brief account. The scattering equations are set up in the laboratory-frame close-coupling approximation (LFCCA) as described by Arthurs and Dalgarno.[17] The details of target wave function and static potential are exactly the same as discussed by Mukherjee, Sur, and Ghosh[10] for the N_2 molecule. For the case of the H_2 molecule, the static potential and density are calculated by using the wave functions of Fraga and Ransil.[18] The static potential is expanded as

$$V_{st}(\mathbf{r}; \hat{\mathbf{R}}) = \sum_{\lambda} v_\lambda(r) P_\lambda(\hat{\mathbf{r}} \cdot \hat{\mathbf{R}}) . \tag{1}$$

In the case of N_2, the terms up to $\lambda = 10$, and for H_2 terms up to $\lambda = 6$, have been retained. In Eq. (1), various terms have the usual meaning (see Ref. 10). The PCOP

potential is obtained from the correlation potential $V_{corr}(\mathbf{r})$ (in atomic units) defined as[6-8], for $r_s \leq 0.302$,

$$2V_{corr}(\mathbf{r}) = \frac{-1.82}{\sqrt{r_s}} + [0.051 \ln(r_s) - 0.115]$$
$$\times \ln(r_s) + 1.167 ; \tag{1a}$$

for $0.302 \leq r_s \leq 0.56$,

$$2V_{corr}(\mathbf{r}) = -0.923\,05 - \frac{0.090\,98}{r_s^2} ; \tag{1b}$$

and for $0.56 \leq r_s \leq 8.0$,

$$2V_{corr}(\mathbf{r}) = -\frac{8.7674 r_s}{(r_s + 2.5)^3} + \frac{-13.151 + 0.9552 r_s}{(r_s + 2.5)^2}$$
$$+ \frac{2.8655}{r_s + 2.5} - 0.6298 . \tag{1c}$$

Here the density parameter r_s is defined as $\frac{4}{3}\pi r_s^3 \rho(\mathbf{r}) = 1$. Finally, we write the $V_{pol}(\mathbf{r})$ as follows:

$$V_{pol}(\mathbf{r}) = V_{corr}(\mathbf{r}), \quad r \leq r_c , \tag{2a}$$

and

$$V_{pol}(\mathbf{r}) = -\frac{\alpha_0}{2r^4} - \frac{\alpha_2}{2r^4} P_2(\cos\theta), \quad r \geq r_c . \tag{2b}$$

Here r_c is radial point where the PCOP potential and the asymptotic form [Eq. (2b)] cross each other for the first time. The values of α_0 and α_2 for H_2 (N_2) targets used here are 5.53 (11.74) a_0^3 and 1.41 (3.17) a_0^3, respectively.

The LFCCA scheme has retained six rotational ($j = 0,2,4,6,8,10$) states for both the targets. The LFCCA equations have been solved for up to the total angular
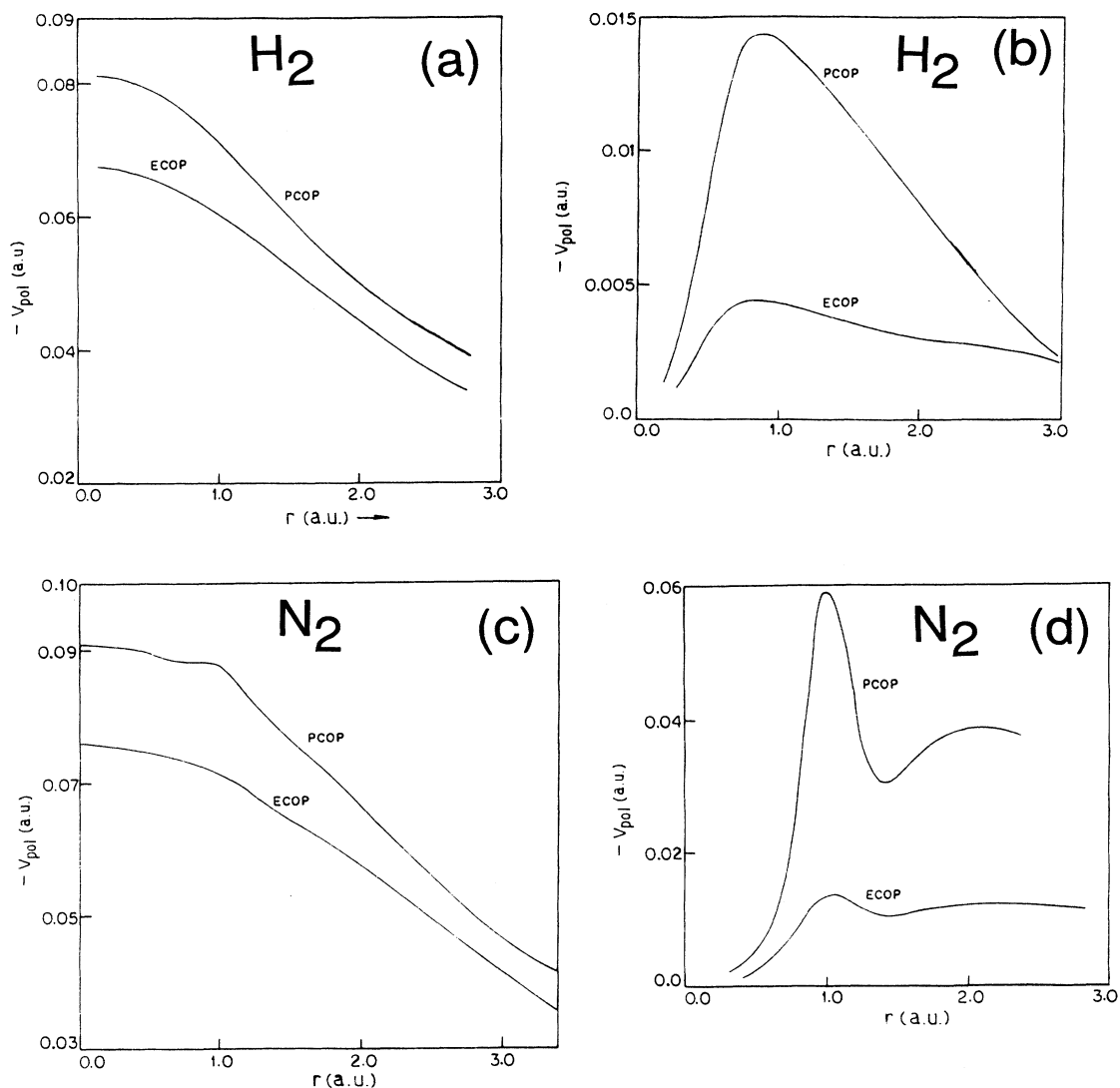

FIG. 1. PCOP and ECOP potentials for H_2 and N_2 targets. The spherical terms are shown by curves in (a) and (c), while non-spherical parts are displayed in figures (b) and (d).
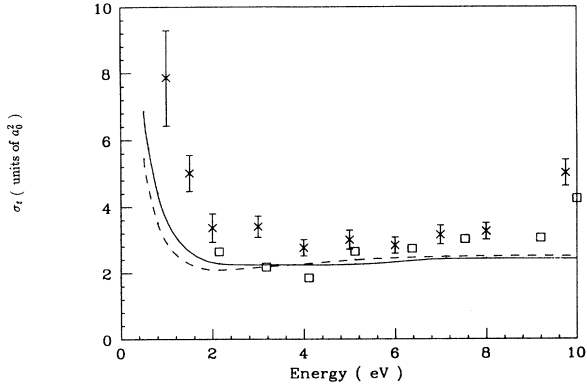
FIG. 2. e^+-H_2 total (rotationally summed) cross section in the PCOP (solid line) and ECOP (dashed line) approximations. The experimental data are from Refs. 19 (crosses) and 20 (squares).

momentum $J=12$ at all energies considered here. The differential equations were integrated using the variable step-size Numerov method with starting step size of $0.001a_0$. We used a value of $120.0a_0$ for the maximum radial distance for integration purpose.

Figure 1 displays the electron-correlation-polarization (ECOP) and PCOP potentials for both targets for both the spherical and nonspherical terms [Eq. (2)]. We see a significant difference between the two approximations as expected. The PCOP model is much stronger than the corresponding ECOP one. This is the case for all other atomic and molecular cases studied so far under the PCOP model.[6-8]

First we discuss our H_2 cross section as shown in Fig. 2 along with the experimental data. The PCOP approximation improves over the ECOP one below 3 eV. Above 3 eV, the models are quite close to each other. Below 2 eV, our PCOP σ_t values are still lower by about a factor of 2 relative to the measured values of Charlton et al.[19] Table I gives the σ_t values in the PCOP approximation. In Fig. 3, the σ_t values for the e^+-N_2 case in the PCOP and ECOP models are shown along with the experimen-

FIG. 3. Same as in Fig. 2, but for the e^+-N_2 system. The lower figure (b) compares PCOP and ECOP values below 1 eV.

tal points.[19,20] In Fig. 3(b), we have shown the same theoretical results below 1 eV energy. As seen earlier for the H_2 case, at lower energies, the PCOP values are higher than the corresponding ECOP results. It is clear from Fig. 3(a) that the PCOP approximation is better

TABLE I. Rotationally elastic, inelastic, and summed cross sections (in units of a_0^2) for the e^+-H_2 collision using static plus PCP polarization potential. For notations see the text.

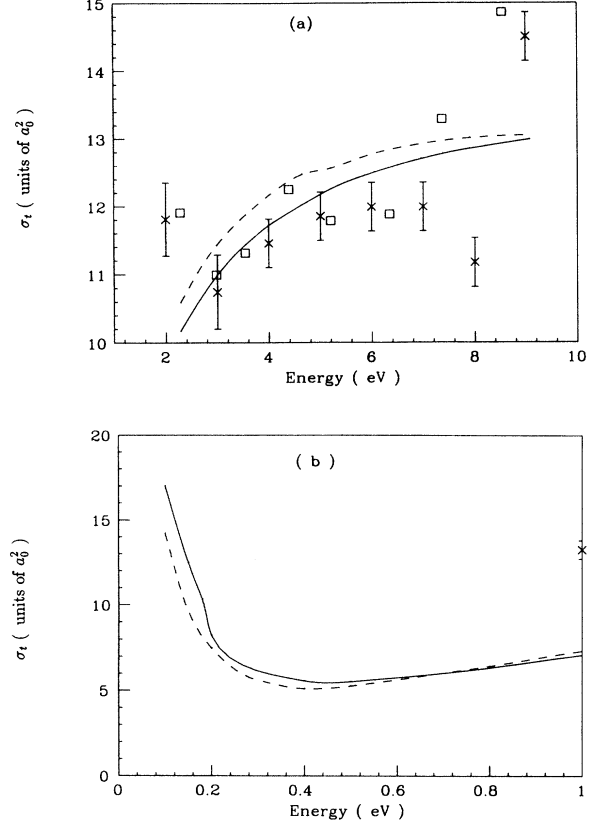| E (eV)	$0\rightarrow0$	$0\rightarrow2$	$0\rightarrow4$	Total summed
0.50	6.645	0.206	0.000 001 7	6.85
0.6	5.591	0.208	0.000 002	5.799
0.8	4.206	0.210	0.000 003 1	4.417
1.0	3.38	0.211	0.000 004 2	3.591
2.15	2.059	0.217	0.000 014	2.276
3.41	2.02	0.221	0.000 033	2.241
5.12	2.123	0.226	0.000 076	2.349
7.12	2.183	0.230	0.000 198	2.413
8.0	2.190	0.232	0.000 187	2.422
10.07	2.178	0.237	0.000 289	2.415

TABLE II. Same as in Table I but for the e^+-N_2 system.

E (eV)	$0\rightarrow0$	$0\rightarrow2$	$0\rightarrow4$	Total summed
0.10	12.70	4.25	0.000 13	16.95
0.20	6.85	1.36	0.001 3	8.221
0.40	4.18	1.37	0.001 45	5.551
0.50	4.13	1.37	0.002 3	5.502
0.80	5.14	1.16	0.005 1	6.305
1.00	6.01	1.05	0.006 3	7.066
2.28	9.66	0.500	0.002 81	10.163
2.98	10.60	0.359	0.004 1	10.963
3.54	11.10	0.302	0.005 1	11.407
4.08	11.40	0.270	0.005 86	11.676
4.64	11.70	0.258	0.006 6	11.965
5.20	11.90	0.259	0.007 2	12.166
6.05	12.20	0.277	0.007 8	12.485
6.96	12.30	0.312	0.008 1	12.62
7.90	12.4	0.360	0.008 24	12.768
9.07	12.5	0.429	0.008 2	12.937

than the ECOP one. The numerical data of Fig. 3 are given in Table II.

Next we show our rotationally inelastic $(0 \rightarrow 2$ only) $\sigma_t^{0 \rightarrow 2}$ cross sections for the e^+-N_2 case at low (below vibrational threshold) energies in Fig. 4. At higher energies (not shown in Fig. 4), the two models are almost identical. In this threshold region, the approximation involved in the polarization potential makes substantial changes in the rotational excitation mechanism. The PCOP model gives the threshold peak much stronger and closer to the threshold as compared to the ECOP model. It may be interesting to compare these results (Fig. 4) with the observation of Coleman, Griffith, and Meyland,[21] who have approximately estimated the cross sections for the rotational excitation in the e^+-N_2 scattering. The position of the threshold peak seems to be below 0.05 eV as is the case in our PCOP model (Fig. 4). We emphasize that our PCOP values for the rotational excitation cross sections of N_2 molecules by low-energy positrons (given in Table II) may be quite useful in experimental analysis.

Finally, we conclude that the present PCOP model to include polarization effects in e^+-molecule collisions is quite promising. We emphasize that a true positron polarization potential must be employed rather than a potential taken as such from the electron-scattering case. In the threshold region, the rotational excitation process is very sensitive to the polarization effect.
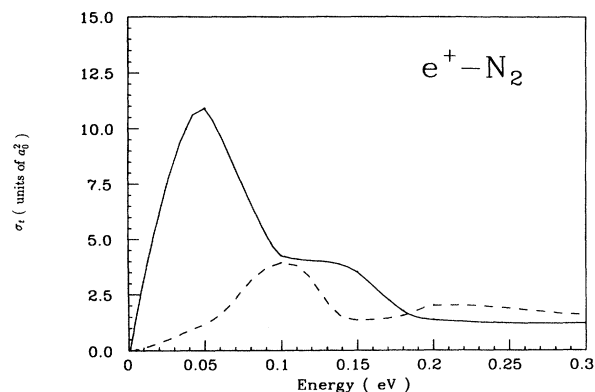

FIG. 4. Rotationally inelastic cross sections in the PCOP (solid curve) and ECOP (dashed line) models for the quadrupole $(j=0$ to 2) transition in the e^+-N_2 case.

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