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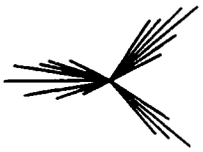

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Proton-positronium-atom scattering in the close coupling approach *

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We present results for low-energy elastic and capture cross sections for proton-positronium-atom scattering with three different basis sets using the close coupling approach. A sharp resonance is found in the elastic channel employing the four-state [H(1s,2s,2p) and Ps(1s)] expansion basis, just above the scattering threshold, at an incident positronium-atom energy of 0.0486 eV. Resonances are also found in the capture cross sections to H(1s), H(2s), and H(2p) states in different partial waves.

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We study low-energy proton-positronium-atom scattering in the close coupling approximation (CCA). The proton-positronium-atom system is a three-particle system with some unique interesting properties, which makes this study of general theoretical interest. First, this is the simplest three-particle system, where the particles are distinguishable and no effect of antisymetrization is needed. Second, the Born term for the elastic proton-positronium-atom scattering in the CCA vanishes and the static elastic cross section is identically zero. Consequently, the elastic scattering in the multistate CCA proceeds via coupling to other channels. Third, this is the simplest system where an exotic channel is open right at the scattering threshold, e.g., the hydrogen formation channel. Finally, we find many resonances in this system both in the elastic and rearrangement cross sections. So a controlled study of the proton-positronium-atom system should reveal interesting physics of positron and positronium-atom interaction with atoms and this system should provide a theoretical laboratory for improving our understanding of the low-energy positron physics. Such a study should also reveal the effect of coupling to other rearrangement channels including an exotic channel, or the origin of resonances, etc. Being a very heavy particle the proton is considered fixed in the center-of-mass frame which significantly simplifies the mathematical treatment.

Neutral atoms can be used as probe of solid surfaces. Because of the smaller mass of the positronium atom it has much larger velocity than an ordinary atom for a given energy. So positronium atom is now considered to be a better probe of solid surfaces than usual neutral atoms. Scattering involving positronium atoms, as in the present Letter, should reveal the interaction of positronium atom with matter, which should be of value in probing solid surfaces. Also, with the recent availability of good quality monoenergetic positronium beam, proton-positronium-atom scattering seems feasible in the future, which will make this study of interest to experimentalists too.

The CCA provides a practical framework for dealing with electron-atom and positron-atom scattering. Unlike the variational calculations[1], CCA deals with rearrangement and elastic channels in an unified way and provides results for elastic and transition cross sections. This approach has been frequently used in e^+-H and other positron-atom scattering[2–10].

We shall use the following basis sets in the present study:

(A) Ps(1s)+H(1s),

(B) Ps(1s)+H(1s,2s), and

(C) Ps(1s)+H(1s,2s,2p),

where Ps denotes the positronium atom and H the hydrogen atom. The model (A) is the usual coupled static model, the model (B) is the present three-state model and the model (C) is the present four-state model. Unlike in the positron-hydrogen-atom scattering, the static model employing only the Ps(1s) state leads to a null Born term and hence to triviallity.

We calculate the elastic cross section for proton-positronium-atom scattering and different transition cross sections to the 1s, 2s, and 2p states of the hydrogen atom in the S, P, and D angular momentum states. We find resonances in some of these cross sections. The real part of the eigen-phase shift for the S-wave elastic scattering exhibits a sharp resonance at an incident positronium-atom energy of 0.0486 eV.

The four- (three-, two-) state CCA leads to four (three, two) coupled Lippmann-Schwinger-type integral equations [1-5]. The four coupled equations of the four-state CCA can be written schematically in the following form:

$$\begin{pmatrix} T_{Ps,Ps} \\ T_{1s,Ps} \\ T_{2s,Ps} \\ T_{2p,Ps} \end{pmatrix} = \begin{pmatrix} 0 \\ V_{1s,Ps} \\ V_{2s,Ps} \\ V_{2p,Ps} \end{pmatrix} + \begin{pmatrix} 0 & V_{Ps,1s}G_{0,1s} & V_{Ps,2s}G_{0,2s} & V_{Ps,2p}G_{0,2p} \\ V_{1s,Ps}G_{0,Ps} & V_{1s,1s}G_{0,1s} & V_{1s,2s}G_{0,2s} & V_{1s,2p}G_{0,2p} \\ V_{2s,Ps}G_{0,Ps} & V_{2s,1s}G_{0,1s} & V_{2s,2s}G_{0,2s} & V_{2s,2p}G_{0,2p} \\ V_{2p,Ps}G_{0,Ps} & V_{2p,1s}G_{0,1s} & V_{2p,2s}G_{0,2s} & V_{2p,2p}G_{0,2p} \end{pmatrix} \begin{pmatrix} T_{Ps,Ps} \\ T_{1s,Ps} \\ T_{2s,Ps} \\ T_{2p,Ps} \end{pmatrix}. \tag{1}$$

In Eq. (1) Ps denotes the 1s state of the positronium atom, and 1s (2s,2p) denotes the 1s (2s,2p) state of the hydrogen atom; G_0 denotes the Green function for the corresponding propagations. The T's are the transition operators for the transition from the initial Ps-atom channel.

After a partial-wave projection the usual coupled Lippmann-Schwinger-type scattering integral equations of the CCA are:[2, 3, 7]

$$T^J_{\beta\alpha}(\tau'k',\tau k) = B^J_{\beta\alpha}(\tau'k',\tau k) + \frac{1}{2\pi^2}\sum_\kappa \int k''^2 dk'' \frac{B^J_{\beta\kappa}(\tau'k',\tau''k'')T^J_{\kappa\alpha}(\tau''k'',\tau k)}{k''^2 - k^2_\kappa - i0}, \tag{2}$$

with the partial-wave Born term given by

$$B^J_{\beta\alpha}(\tau'k',\tau k) = \frac{(kk')^{1/2}}{2J+1} \sum_{MM_LM_{L'}} \sum_{mm'} < L'l'M_{L'}m'|JM >< LlM_Lm|JM > \times \int d\hat{k}d\hat{k}' Y^*_{L'M_{L'}}(\hat{k}')Y_{LM_L}(\hat{k})B_{\beta\alpha}(\vec{k}',\vec{k}). \tag{3}$$

Here $T^J_{\beta\alpha}(\tau'k',\tau k)$ is the t martix for transition from channel α to β, $B_{\beta\alpha}(\vec{k}',\vec{k})$ is the relevant Born term, k and k' are the relevant wave numbers, L and M_L are the orbital angular momentum and the projection of the relative motion, l and m are the angular momentum and the projection of the atomic states, and τ stands for the collective quantum numbers (n,l,m) of the atomic states, n being the principal quantum number. The off-shell matrix elements for all the Born terms are included in the calculation.

The Lippmann-Schwinger-type coupled integral equations (2) are solved numerically without further approximations by the standard matrix inversion technique [2, 3, 11]. The integration over the free Green function was separated into its principal value and imaginary parts and typically 30 integration mesh points were used per channel to evaluate the principal value integral.

In Fig. 1 the S-wave eigen-phase shift for elastic proton-positronium-atom scattering is plotted versus the incident positronium-atom energy. Because of the open positron-hydrogen-atom channel the elastic scattering phase shift for proton-positronium-atom scattering is complex right at the scattering threshold. However, the eigen phase shift is real and we have calculated the eigen phase shift for the elastic channel. The most interesting aspect of the present study is the appearance of a sharp S-wave resonance in the four-state model (C), for elastic scattering at an incident positronium-atom energy of 0.0486 eV. This eigen-phase shift quickly increases by π at this energy. Resonances have been reported in other positron-atom systems but never at such a low incident projectile energy[2, 12, 13]. Also, in these other cases usually no channels are open right at the scattering threshold. No resonances are found in the two-state model (A).

We calculate the elastic cross section for proton-positronium-atom scattering and different transition cross sections to the 1s, 2s, and 2p states of the hydrogen atom in the S, P, and D angular momentum states. We find resonances in some of these cross sections.

In Fig. 2 we exhibit the elastic proton-positronium-atom scattering cross sections for the three- and four-state CCA models at various energies. The coupled static elastic cross sections are in reasonable agreement with the three- and four-state results. This demonstrates the very strong influence the H(1s) state has on the elastic proton-positronium-atom channel. Once this state is included the low-energy elastic scattering cross section do not

significantly change with the addition of H(2s) and H(2p) states.

In Fig. 3 we present results for S-, P-, and D-wave capture cross sections to the 1s state of the hydrogen atom for models (B) and (C). In this figure the S-wave capture cross sections are multiplied by 100. In the S-wave H(1s) capture cross sections, resonances are found between incident positronium-atom energies of 60 and 80 eV in the three- and four-state models. The D-wave H(1s) capture cross section also exhibits resonance-like behaviors for incident positronium atom energies less than 10 eV. .

In Figs. 4 (a) and (b) we present results for S-, P-, and D-wave capture cross sections to the 2s state of the hydrogen atom for models (B) and (C). In the S-wave H(2s) capture cross sections, resonances are found between incident positronium-atom energies of 20 and 40 eV in the three- and four-state models. There are some resonance-like behaviors in the P- and D-wave H(2s) capture cross sections as can be seen in Fig. 4 (b).

Finally, in Fig. 5 we present results for S-, P-, and D-wave capture cross sections to the 2p state of the hydrogen atom for the four-state model (C). The S-wave capture cross section has two prominent minima at incident positronium-atom energies of 25 and 72 eV. Similar resonances in the capture cross section has also been found in positron-hydrogen and positron-helium scattering [14].

In conclusion, we have exhibited the strong effect of the H(1s) formation channel on the elastic channel observables in a CCA calculation of the proton-positronium-atom scattering. We have noted a sharp resonance in the S-wave elastic proton-positronium-atom scattering at an incident positronium atom energy of 0.0486 eV. In addition, we have noted several resonances in the different capture cross sections in S-, P-, and D-waves. In particular, S- and D-wave resonances are found in capture cross sections to the H(1s) state; S-wave resonance is also observed in the capture cross section to the H(2s) state. We believe that the present pioneering CCA study of the proton-positronium-atom system will motivate further theoretical and experimental investigations in the future.

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Figure Caption

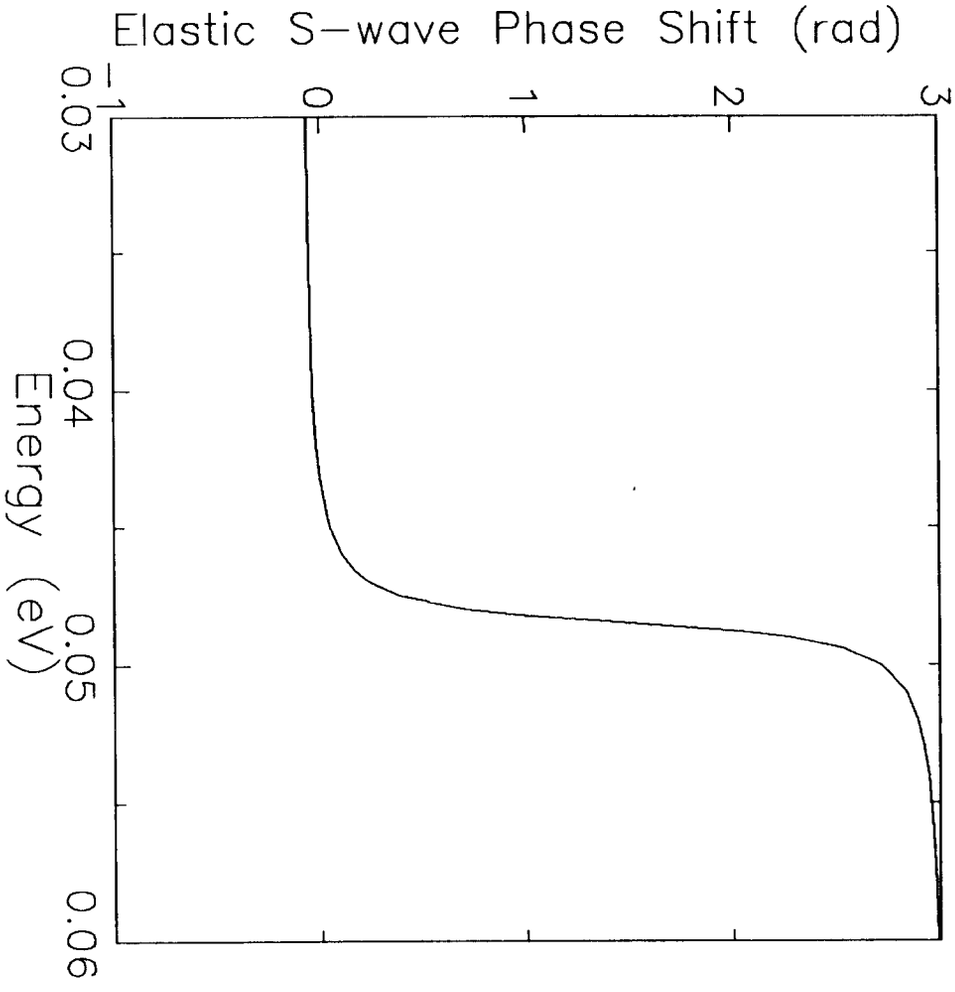
1. S-wave elastic scattering eigen-phase shifts in radians for proton-positronium-atom scattering employing the four-state CCA model (C) at low positronium atom energies.

2. S-, P-, and D-wave elastic proton-positronium-atom scattering cross sections in units of πa_0^2 for the three- and four-state CCA models (B and C) at various incident positronium atom energies, where a_0 is the Bohr radius of the hydrogen atom. The label P-4, for example, denotes results for P-wave four-state CCA calculation.

3. S-, P-, and D-wave capture cross sections to the 1s state of the hydrogen atom in units of πa_0^2 for the three- and four-state CCA models (B and C) at various incident positronium atom energies. The S-wave results are multiplied by 100. Notations are the same as in Fig. 2.

4. (a) S-, (b) P-, and D-wave capture cross sections to the 2s state of the hydrogen atom in units of πa_0^2 for the three- and four-state CCA models (B and C) at various incident positronium atom energies. Notations are the same as in Fig. 2.

5. S-, P-, and D-wave capture cross sections to the 2p state of the hydrogen atom in units of πa_0^2 for the four-state CCA model (C) at various incident positronium atom energies. Notations are the same as in Fig. 2.



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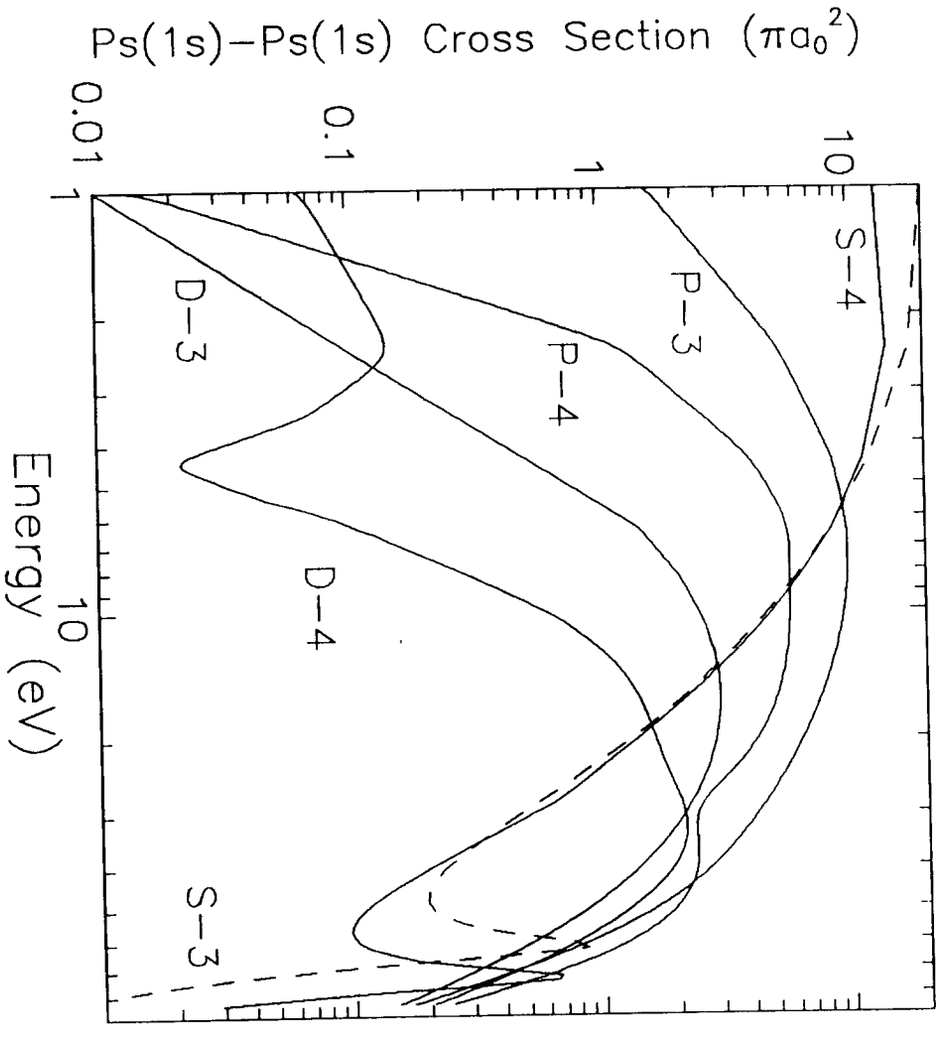

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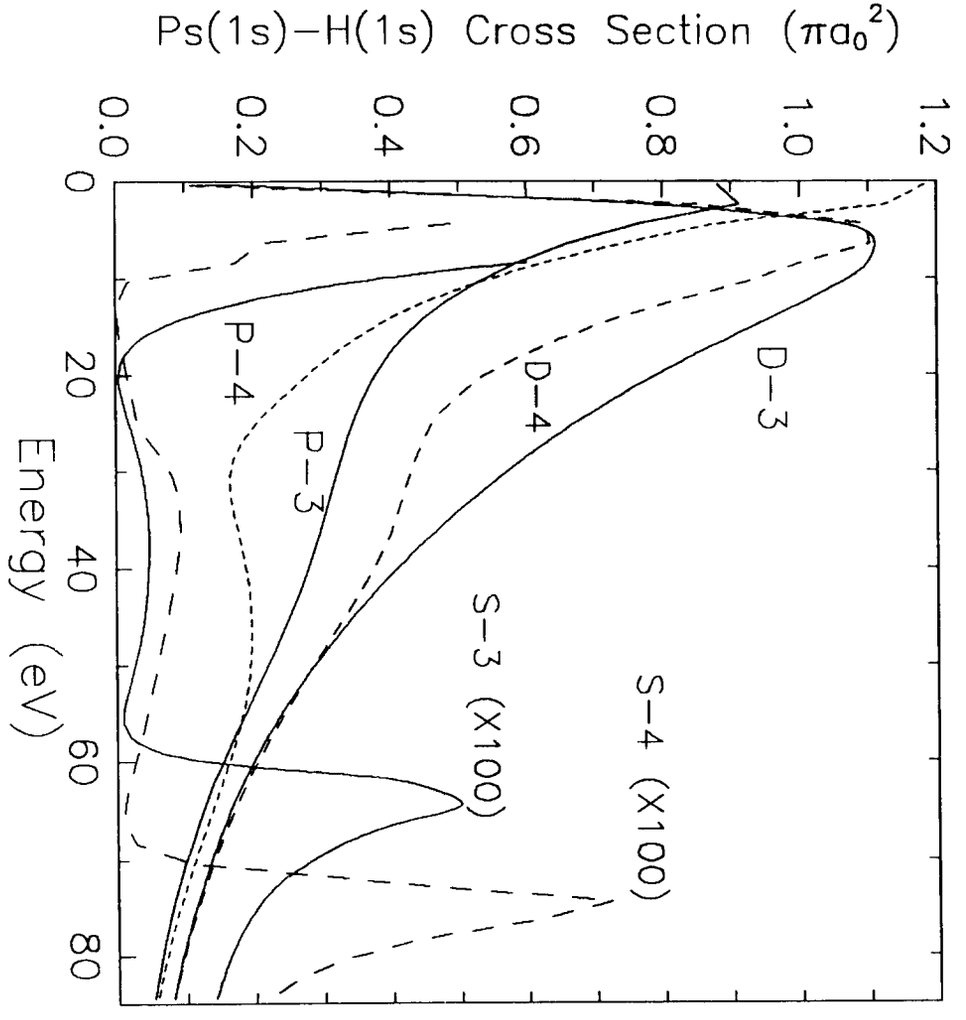

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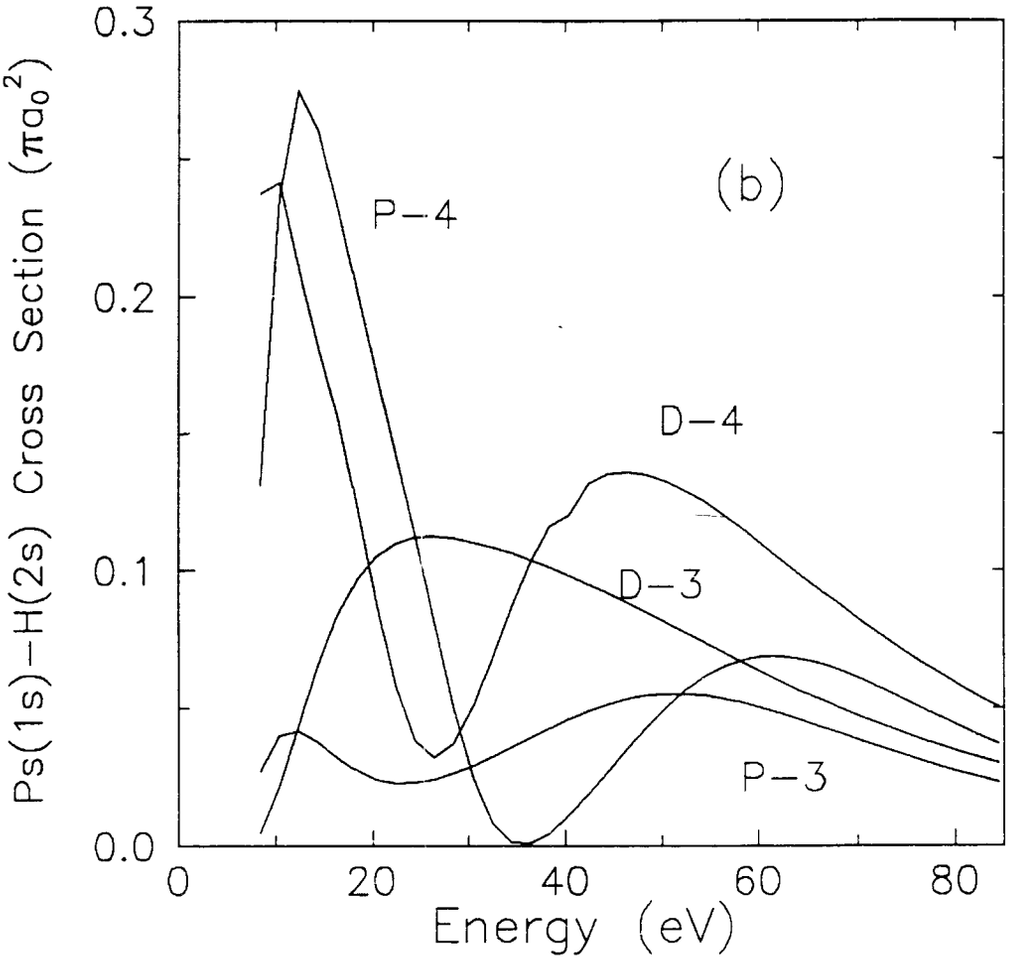

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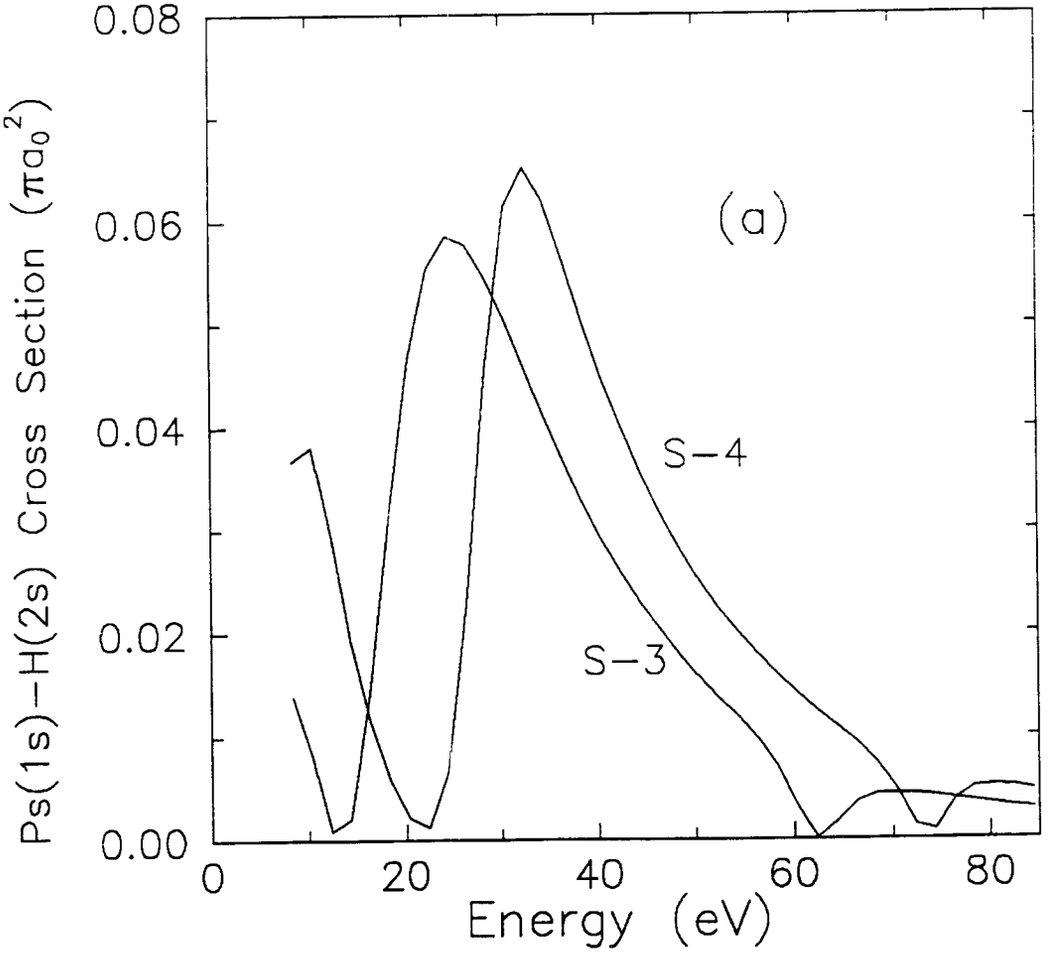

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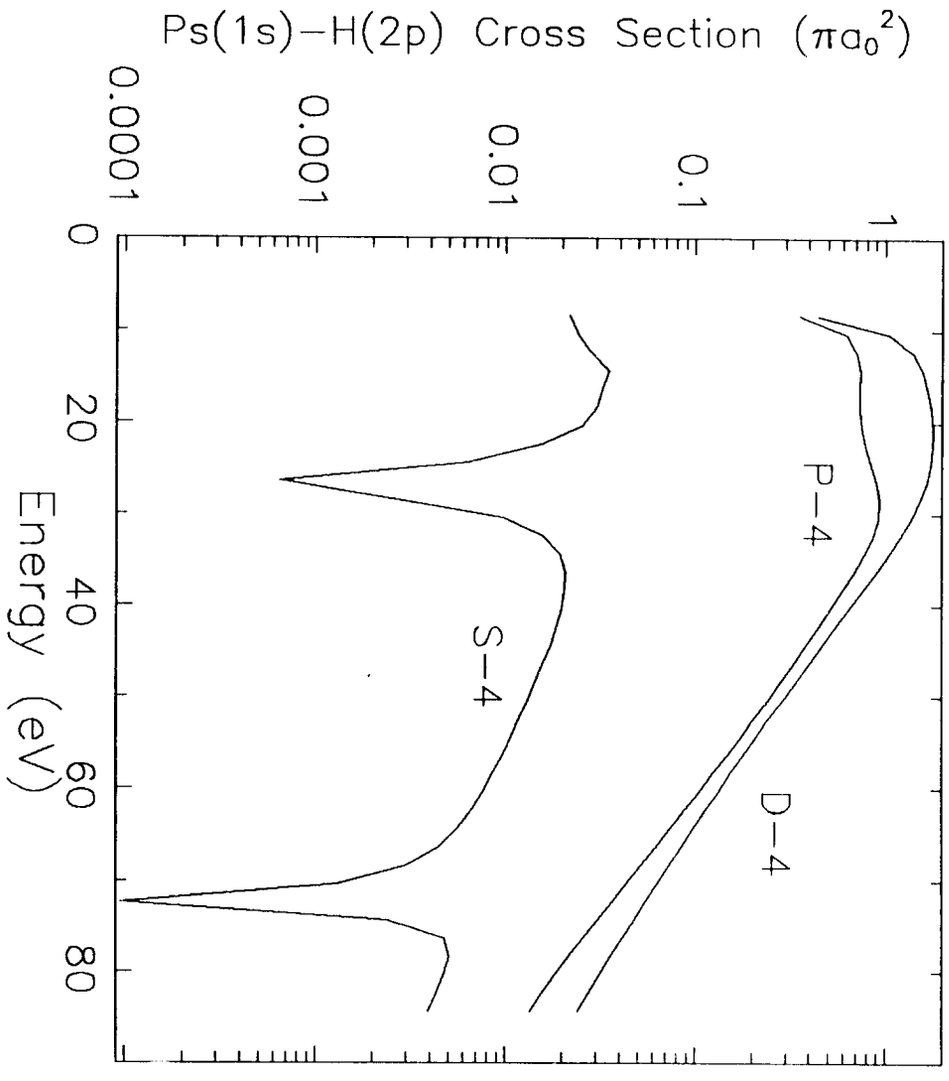

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