# ELASTIC SCATTERING OF POSITRONS BY RARE GASES ATOMS AT LOW AND INTERMEDIATE ENERGIES BY USING MULTIPOLE POLARISABILITY POTENTIAL

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## *Abstract*

We have calculated the phase shifts, differential cross sections (DCS's), total cross sections (TCS's) and momentum transfer cross sections (MTCS's) for the positrons scattered elastically from Ne, Ar, Kr and Xe atoms. The theoretical method is based on combining the static potential with the polarisation potential (containing both dipole and quadrupole polarisabilities) at long distances and with the correlation potential of Ashok Jain at short distances. We found a good general agreement with other experimental and theoretical values of many investigators.

## *1. Introduction*

Noble gases are characterized by a tightly bound, completely filled valence shell, thus they have large ionisation potentials and the elastic scattering, cross section are much larger than the inelastic ones. The dominant interactions in the scattering process are described by the static and polarisation potentials (1).

Experimental measurements for the scattering of positrons by atoms are not only interesting because they involve interactions of antimatter with matter, but also because they can help to provide a better understanding of the scattering of electrons by atoms which are of great importance in many different fields of science and technology such as plasma physics (including fusion research, laser development, gaseous electronics, astrophysics, and aeronomy (2).

The elastic scattering of positrons on rare gas atoms is are of the simplest scattering problems and is therefore suitable for testing different calculational methods (3), since positrons differ from electrons only by the sign of their electric charge, comparison measurements of the scattering of positrons and electrons by atoms can reveal some interesting similarities and differences that arise from the basic interactions contributing to $e^{\pm}$ scattering.

The interaction between a positron and an atom is largely dominated by two opposing interactions. First, there is the coulomb interaction between the positron and the nucleus. This results in a repulsive interaction between the positron and unperturbed atom. This static interaction between the positron and the atom is easy to compute accurately. However, the electronic change cloud of the atom is perturbed whenever there is a positron nearby. The polarization of the electron charge cloud leads to an attractive interaction between the positron and the atom (4).

In one respect, the calculation of e+-atom scattering is simpler than $e^-$ atom scattering. There is no exchange interaction between the positron and target electrons. But in every other respect, the theoretical treatment of $e^+$ atom scattering is a more difficult proposition than $e^-$ atom scattering. The reason for this lies in the attractive nature of the $e^{\pm}$ $e^-$ interaction, which leads to a very strong $e^- e^+$ correlation (5).

Experiments on positron-atom scattering have been reviewed recently by Charlton (6), Raith (7), Stein and Kauppila (8) and Kauppila and Stein (2). The theoretical work on this

subject has been reviewed by McEachran (9), Drachman (10). Schrader and Svetic (11) and Flooder et al., (12).

In our calculations of elastic positron scattering from these gases, we have taken the correlation potential of Jain (13) with polarisation potential of Ali (14) to compsite a new model called correlation polarisation potential model (CPP).

This model yielded very good results for low-energy scattering (i.e. up to a few eV ) but became somewhat less accurate at higher energies for rare gases only.

It is our aim, in this paper, to develop, a model calculation of elastic cross sections for positron scattering which will be applicable throughout the low and intermediate energy regions.

## *2. Model of Calulation*

In the static approximation of the scattering theory starts with solving the Hartree -Fock equation [15,16] (in atomic units: $e^2 = \hbar = m=1$):

$$[-\frac{\nabla_1^2}{2}-\frac{Z}{r_1}+\sum_j\int\frac{U_j^s(2)U_j(2)}{r_{12}}dv_2-\frac{\sum_j\int\delta_{ij}\int U_i^s(1)U_j^s(2)U_i(1)U_i(2)/r_{12}}{U_j^s(1)U_i(1)}]U_i(1)=E_iU_i(1) \quad .....(1)$$

Where the third term on the left represents the Hartree potential, while the last term on the left is the exchange term which is neglected.

In this paper, our goal is to look for a computionally simple form of the positron polarisation potential, the present positron polarisation potentials are based on the correlation energy of a localized positron in an electron gas and its hybridization with correct asymptotic form of Jain (13) as:

$$V_{pol}(r)=\begin{bmatrix} V_{cor}^{SR} & r\le r_0 \\ V_{pol}^{LR} & r>r_0 \end{bmatrix} \quad .....(2)$$

where $r_0$ is the crossing point between $V_{cor}^{SR}$ (r) and $V_{pol}^{LR}$(r) , $V_{cor}^{SR}$ (r) and is the correlation potential at a distance and $V_{pol}^{LR}$(r) is the polarisation potential at a long distance which is usually taken as (14):

$$V_{pol}^{LR}(r)=-\frac{1}{2}\sum\frac{\alpha_{2L}(0)r^{2L}}{(r^2+d_n^2)^{2L+1}} \quad .....(3)$$

where, $\alpha_{2L}(0)$ are the static multipole polarisabilities of the target and $d_n$ is the cut-off distance of the order of atomic size (n= 1,2,3...). These values of $d_n$ are obtained in our calculation to satisfy $V_{pol}^{LR}(r_0) = V_{cor}^{SR}(r_0)$.

In eq.(3) the value of d is usually used to determine $r_0$ this makes the value $r_0$ dependent on the number of terms included in eq. (3), in this section we present a model of calculation that goes around this problem. The correlation potential of Jain (13) in terms of functional derivative of the density parameter (17) is:

$$2Vcor(r) = \begin{bmatrix} (-1.82)/(\sqrt{r_s}) + [0.05inr_s - 0.115]inr_s + 1.167 \\ \qquad\qquad\qquad\qquad\qquad\qquad for \quad rs \le 0.302 \\ -0.92305 - (0.09098)/(r_s^2) \quad for \quad 0.302 \le rs \le 0.56 \\ (8.7674 \quad r_s)/(r_s + 2.5) - 0.6298 \quad for \quad 0.56 \le r_s \le 8.0 \end{bmatrix} \text{.....(4)}$$

$$where, r_s = [(3)/(4\pi\rho(r))]^{1/3}$$

In figure (la, b), we plot the calculated as a function of the radial distance r. It is shown that $V_{cor}^{SR}$ is a rapidly varying function of r at a very short region (core region), and by increasing r this variation becomes more moderate until a region of r that lies outside the ionic radius where the variation of $V_{cor}^{SR}$ (r) is very low. Inside the latter region, our function behaves linearly with r. Figure (2 a,b) shows the point of minima $r_0$. The details are explained in previous papers (18).

Figure (3a) shows the variation of $V_{st}$ , $V_{pol}$ $V_{cor}$, and $V_{opt}$ as a function of radial distance r for argon - atom, while figure (3b ) shows the variation of $V_{opt}$ (r) as a function of radial distance r for inert gas atom; it is clear that the point $r_0$ increased with increasing the atomic number Z.

We have used the Hartree-Fock wave function given by Clementi and Roetti (19), also we have applied the partial wave method by using CAVLEED program (Titterington and Kinniburgh (20) modified to optimize step sizes) in calculating phase shifts and differential cross sections up to nine phase shifts.

## *3- Results and Discussion*

For rare gases atoms and for dipole and quadrupole polarisabilities, we take $\alpha_2(0)$= 2.66(Ne), 11.07 (Ar), 16.73 (Kr), and 27.26 (Xe) as given by Miller and Bederson (21) and $\alpha_2(0)$= 6.41 (Ne), 50.13 (Ar), 94.33 (Kr),and 204.37 (Xe) as given by Johnson et al. (22) (all quantities in a.u.)

In figure(la), we show the crossing points for Ne, Ar, Kr and Xe atoms are $r_0$ =1.27, 1.91, 2.166 and 2.422 respectively (all these quantities are in atomic units). We show that the positron is expected to distort the target charge cloud deeper due to strong positron-lectron_correlation. Also the local real optical potential Vopt(r) for the e+- system is displayed in Figure (3a) which is a sum of repulsive static $V_{st}$(r) and attractive polarisation Vpol(r) potentials.

Our theoretical phase shifts using the Jam correlation potential (13) are shown in figures (4 a, b, c, d) for positron-Ne, Ar, Kr and Xenon scattering.

These results are compared to other values of Schrader (23), Stein et al. (24), McEachran et al. (25). Figures (5, 6,7,8) are show the results of the differential cross sections for elastic scattering of $e^+$ from Ne, Ar, Kr and Xe for various incident energies. For these results, we compared our results of Ar-atom with the theoretical values of Jain (13), Sjenkiewicz (3), Bartschat (1) and experimental values of Coleman et al. (26), Kauppila et al. (27), Floeder et al. (28), Smith et al. (39), Hyder et at. (30), also figure (1) explains our results for Kr-atoms with theoretical values of Szmytkowski (31) and experimental values of Dou et al. (32). Also DCS's are calculated for e scattering for incident energy 40 and 100 eV in figure (8). These are compared with other theoretical calculations of Hasenburg et al. (33).

The results of the present data of the total elastic scattering are shown in figure (9a) for neon atom, our results are compared to the theoretical values of McEachran et al. (25) and experimental values of Chariton et al. (34), Kauppila et al. (35) and Canter et al. (36). Our calculation of Ar-atom in figure (9b) is compared with McEachran et al. (37) and Massey et al. (38) theoretically and with Chariton et al. (34), Kauppila et al. (35) and Canter et at. (36) experimentally, while our data of Kr-and Xe-atom are compared with theoretical values of

McEachran et a!. (40) and experimental values of Sinapius et al. (40) and Canter et at. (36) as shown in figures (9c,d).

Figure (10) shows momentum transfer cross sections for Ne, Ar, Kr and Xe atoms. Our calculations do not include relativistic effects and we expect that better results will be obtained by including these effects. As a conclusion, we can see that using the correlation potential performed by Jain (13) combined together with parameter free polarisation potential for large atoms with larger polarisabilities can give quite reliable results as we have pointed out for Ne, Ar, Kr and Xe-atoms. Also figures (11a , b) show the total cross sections and momentum transfer cross sections respectively. We note that, if the atomic number increases total cross sections increase at low energies as shown in figure (11 a), figure (11 b) shows Ramsauer maximum. We conclude that the scattering particles increase with increasing the atomic number of atoms.

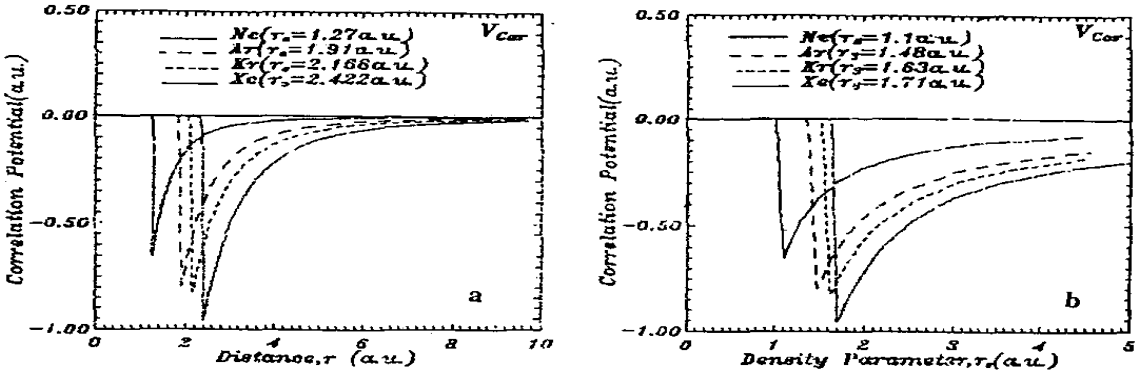


**Fig. (1 a ): Correlation potentials of Ne, Ar, Kr and Xe-atoms as a function of radial distance r.**

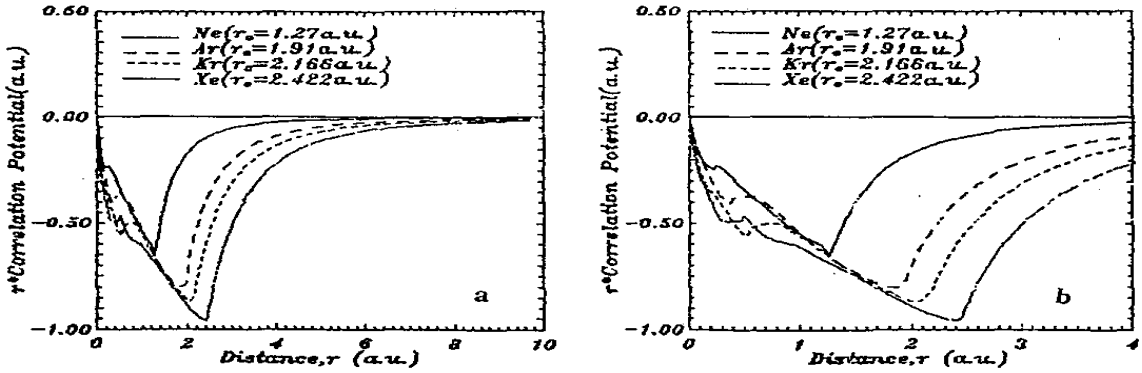


**Fig. (2 a,b): Variation of r Vcor (r) as a function of radial distance r, for rare gases atoms (Ne, Ar, Kr, and Xe).**

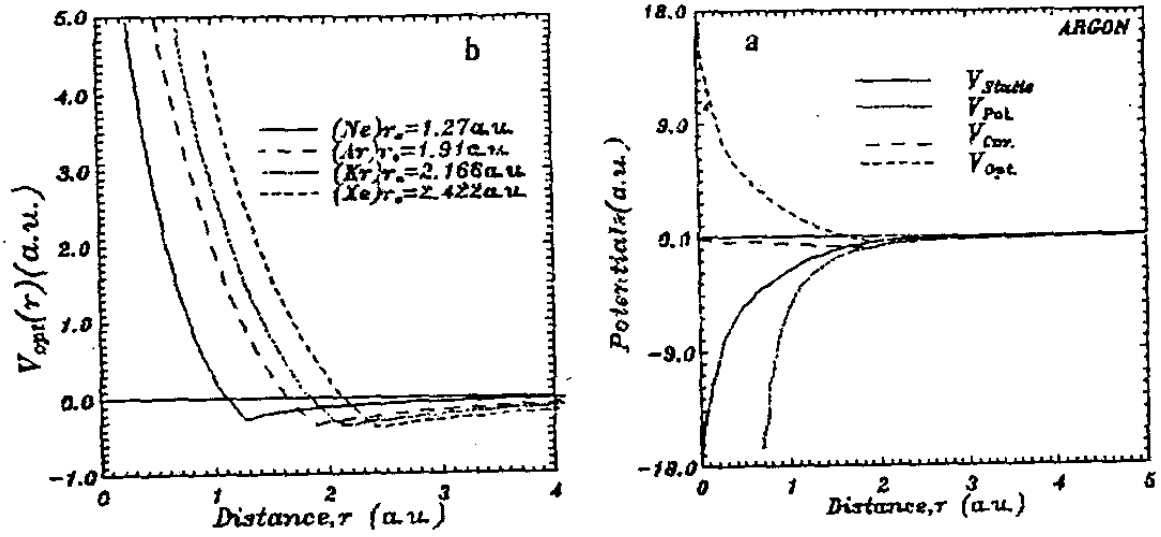


Fig. (3a):Variation of potentials $V_{st}$, $V_{pol}$, $V_{cor}$, $V_{opt}$. with radial distance r.

Fig. (3b):Variation of optical potentials as a function of radial distance r.

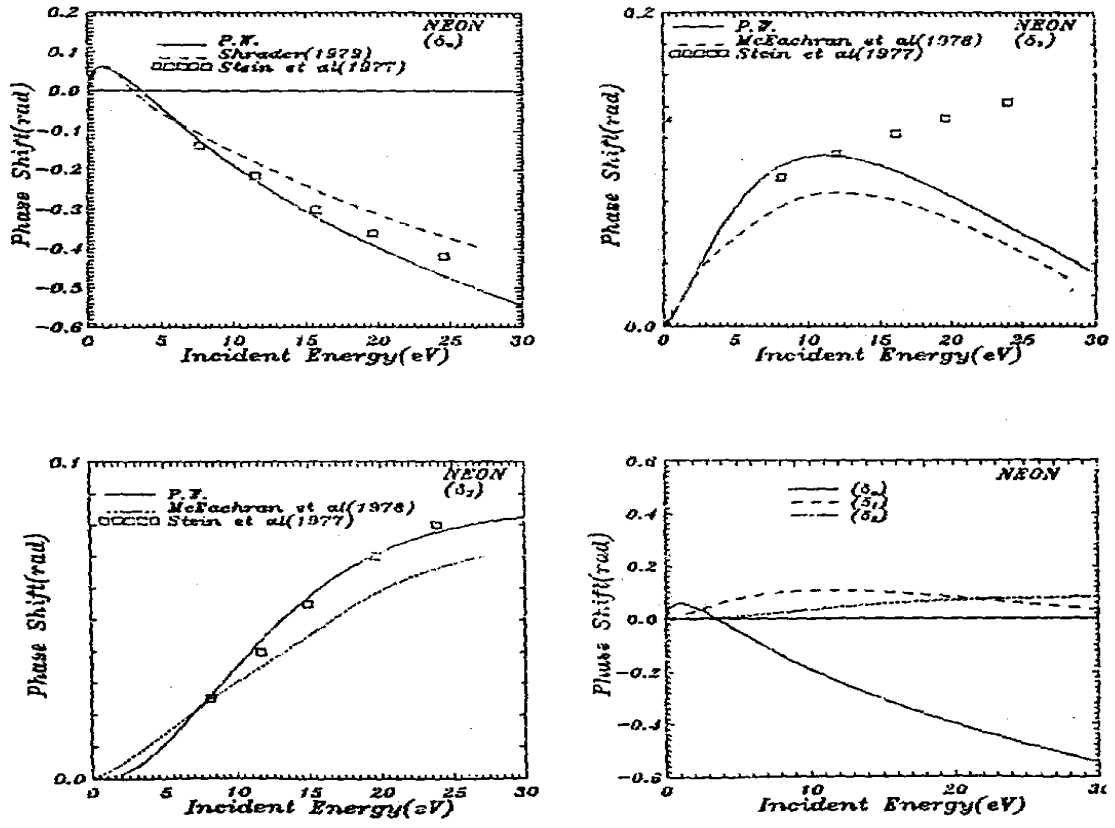


**Fig.4a:** **Phase shift (in rad) for elastic scattering of positrons from neon for s-, p- and d- waves.**

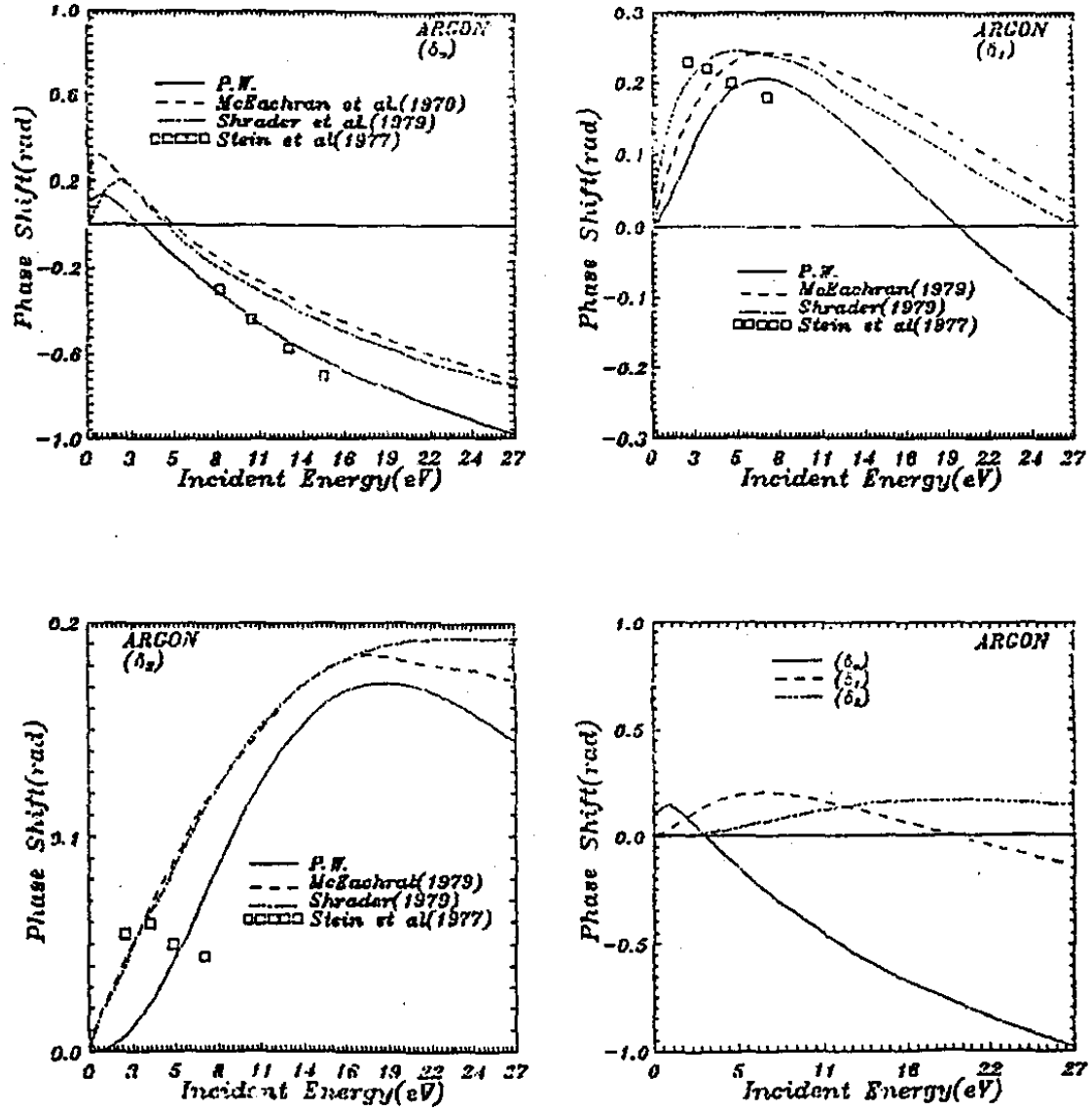


**Fig.4b:** Phase shift (in rad) for elastic scattering of positrons from argon for s-, p- and d- waves.

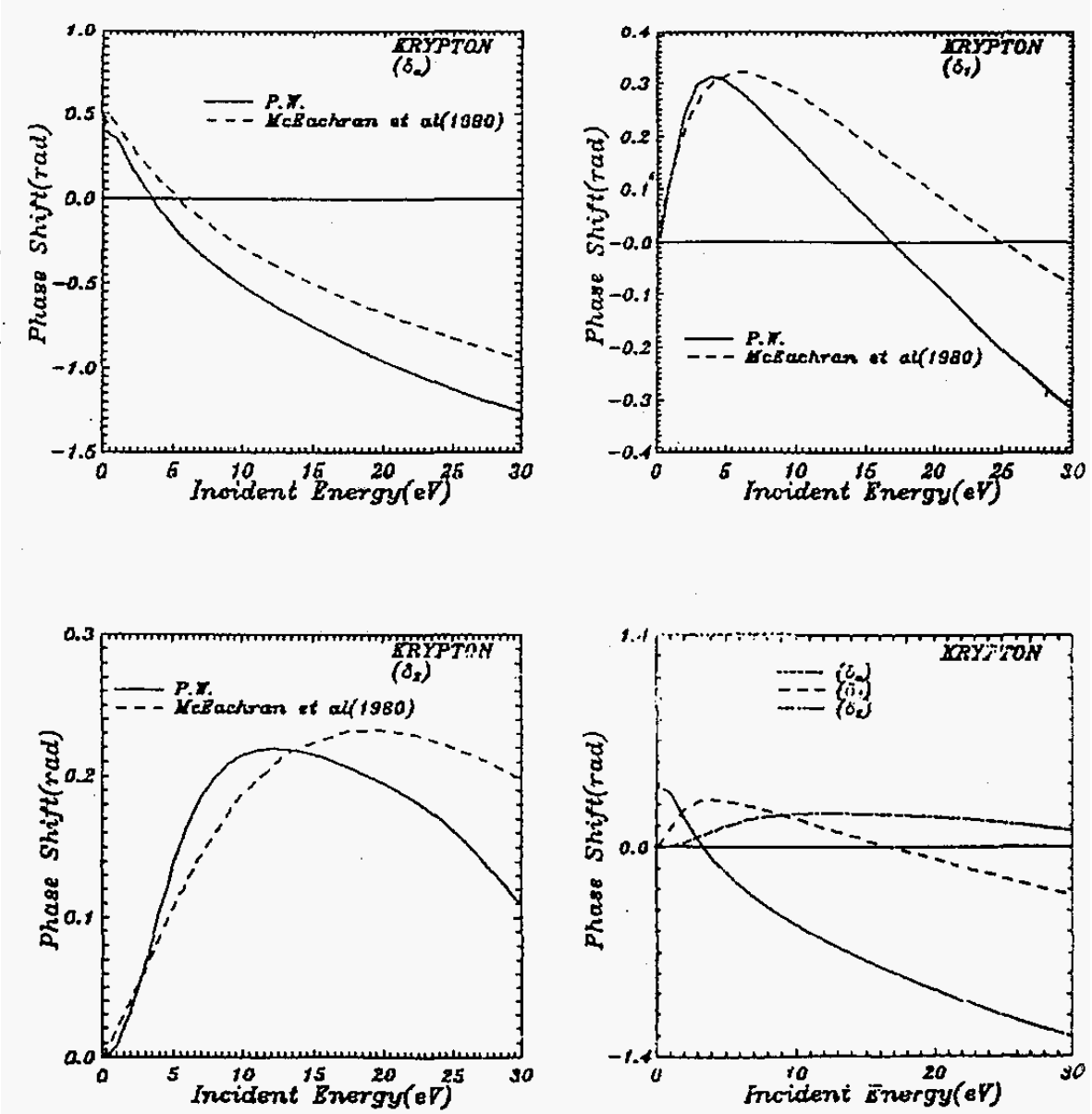


Fig.4c: Phase shift (in rad) for elastic scattering of positrons from krypton for s-, p- and d- waves.

xenon for s-, p- and d- waves.

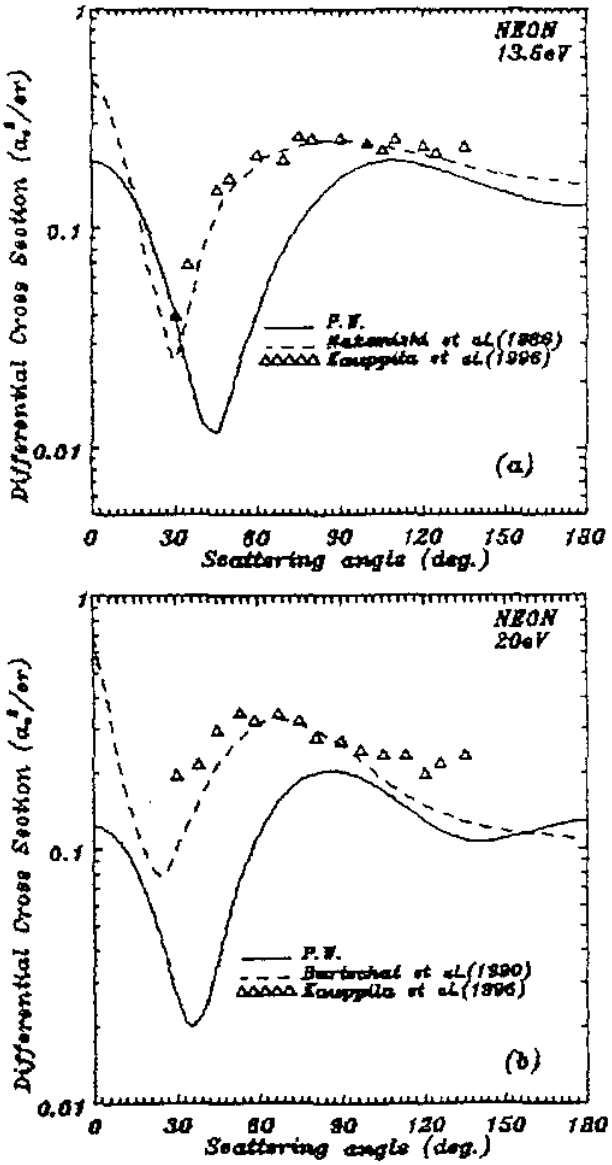


**Fig. 5: Differential cross sections ( $a_0^2$ /sr ) for the elastic scattering of positron from Ne – atoms for incident positron energy (a) 13.6 eV ( b ) 20 eV.**

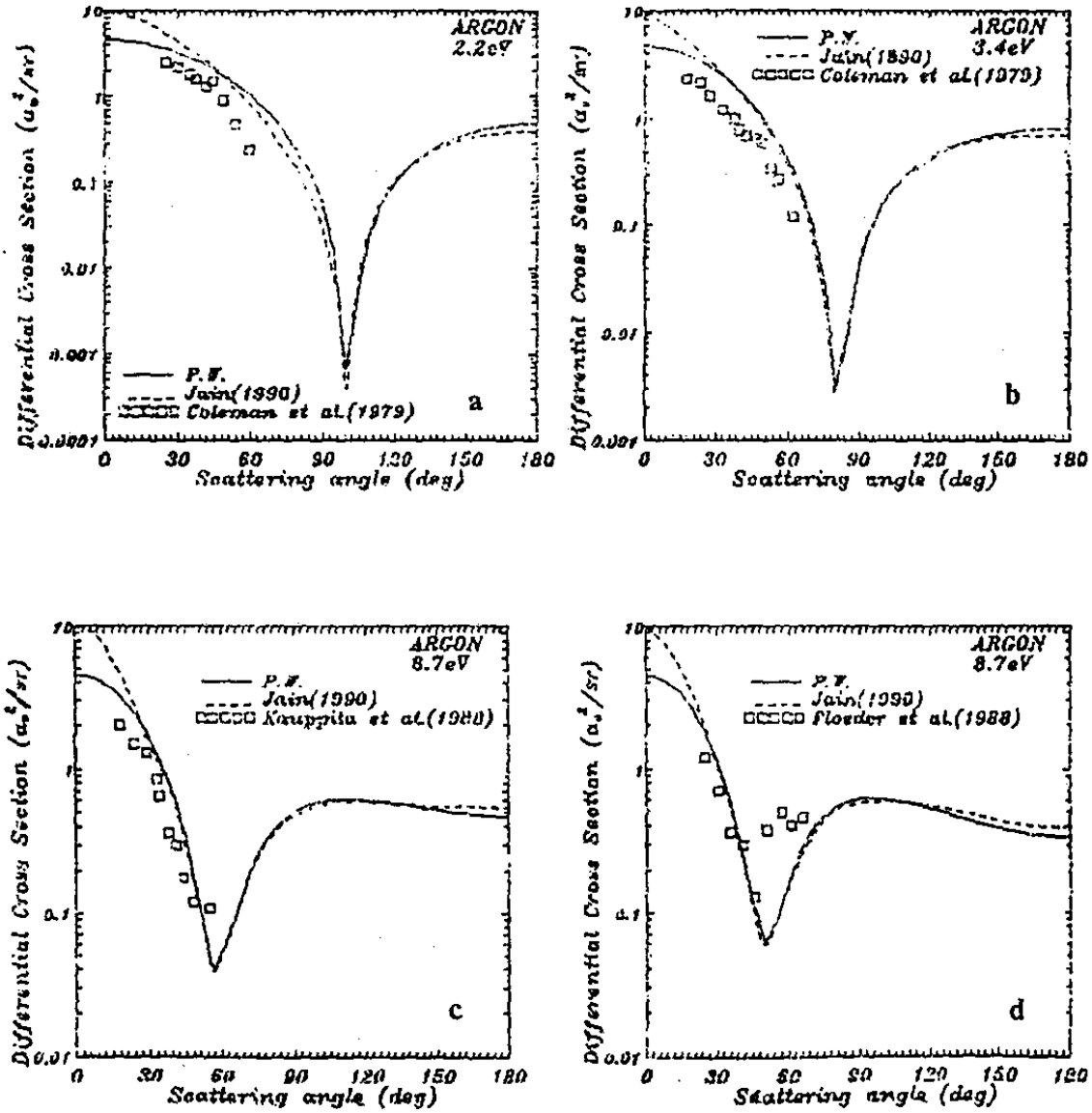


**Fig.6: Differential cross sections ( $a_0^2$ /sr ) for the elastic scattering of positron from Ar – atoms for incident positron energy (a) 2.2eV, ( b ) 3.4 eV ,( c ) 6.7 eV, (d) 8.7 eV, (e) 15 eV,(f)20 eV,(g)30 eV (h)100 eV.**

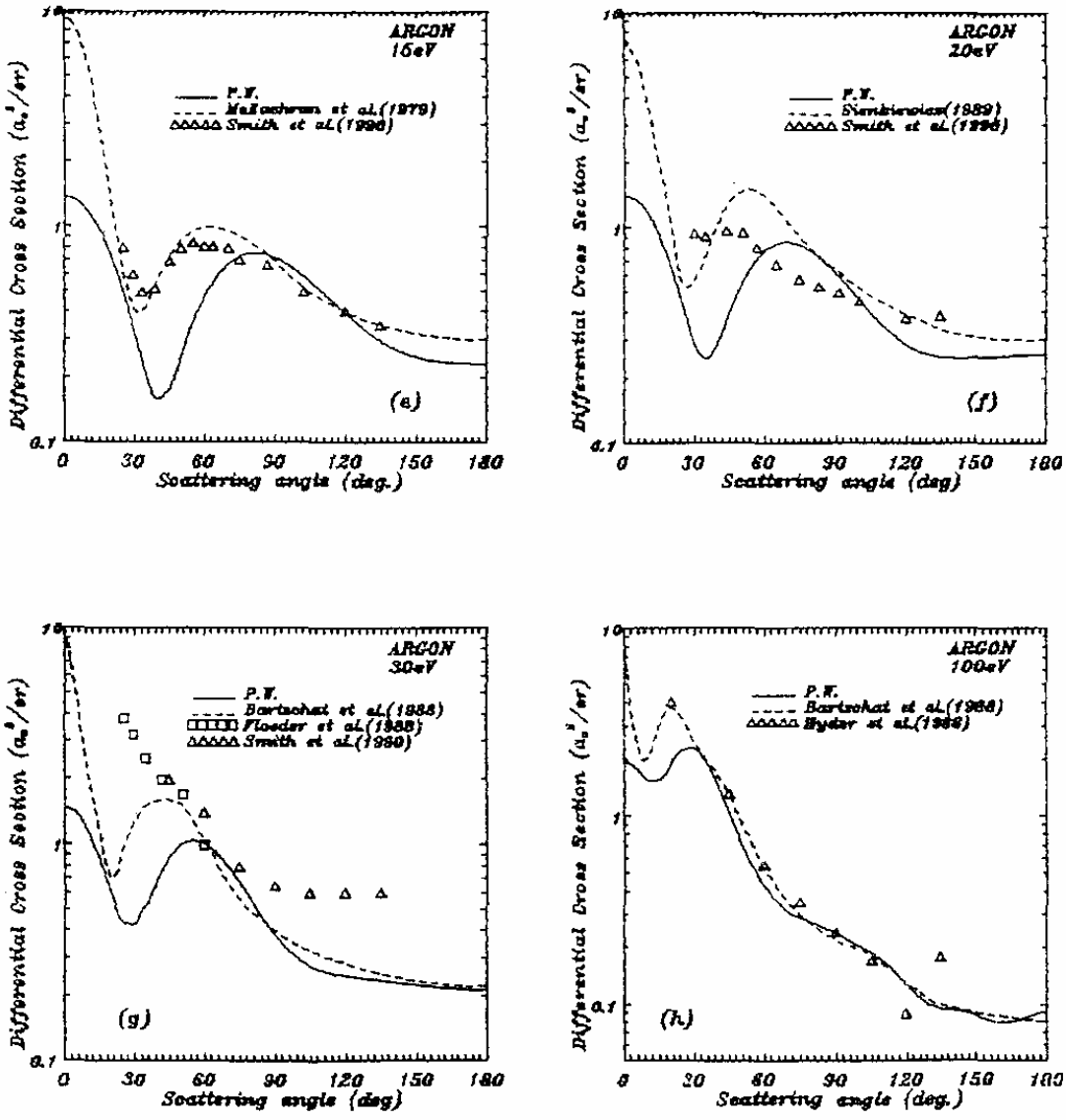


**Fig.6: Continued**

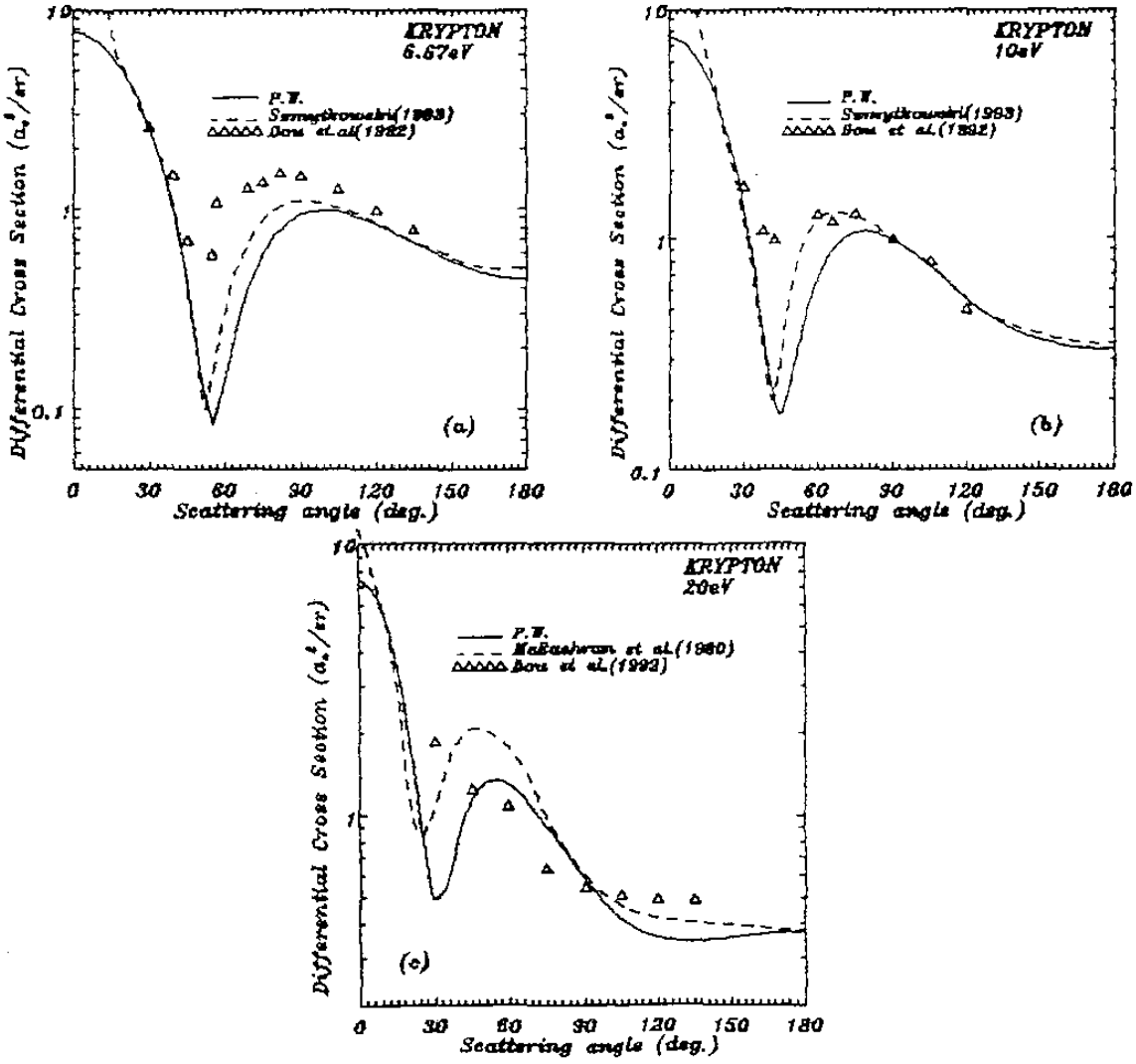


**Fig7: Differential cross sections ( $a_o^2$ /sr ) for the elastic scattering of positron from Kr – atoms for incident positron energy (a)6.67 eV, ( b ) 10eV ,( c )20 eV.**

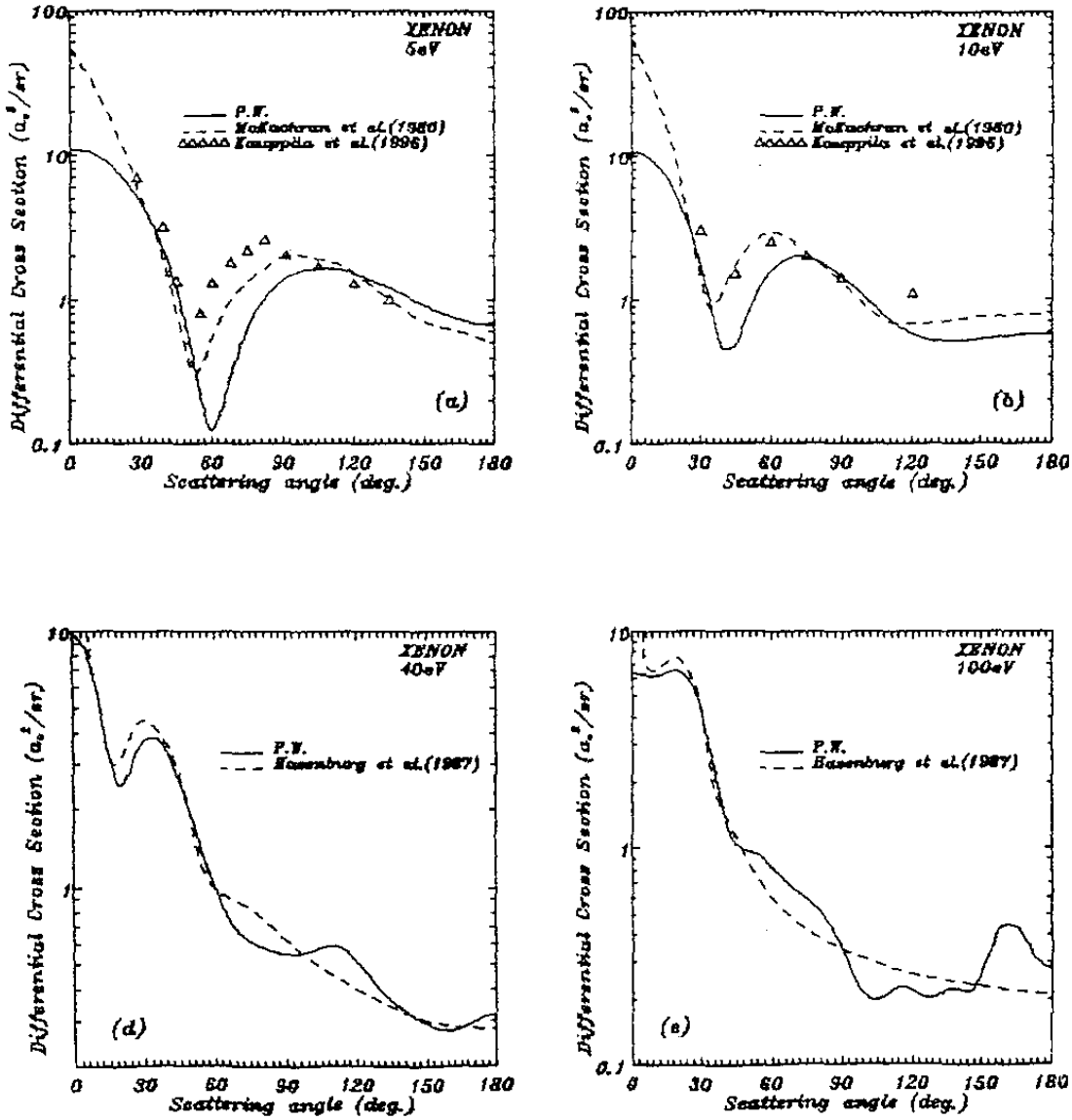


**Fig.8: Differential cross sections ( $a_0^2$ /sr ) for the elastic scattering of positron fromXe – atoms for incident positron energy (a)5eV, ( b ) 10 eV ,( c ) 40 eV, (d) 100 eV.**

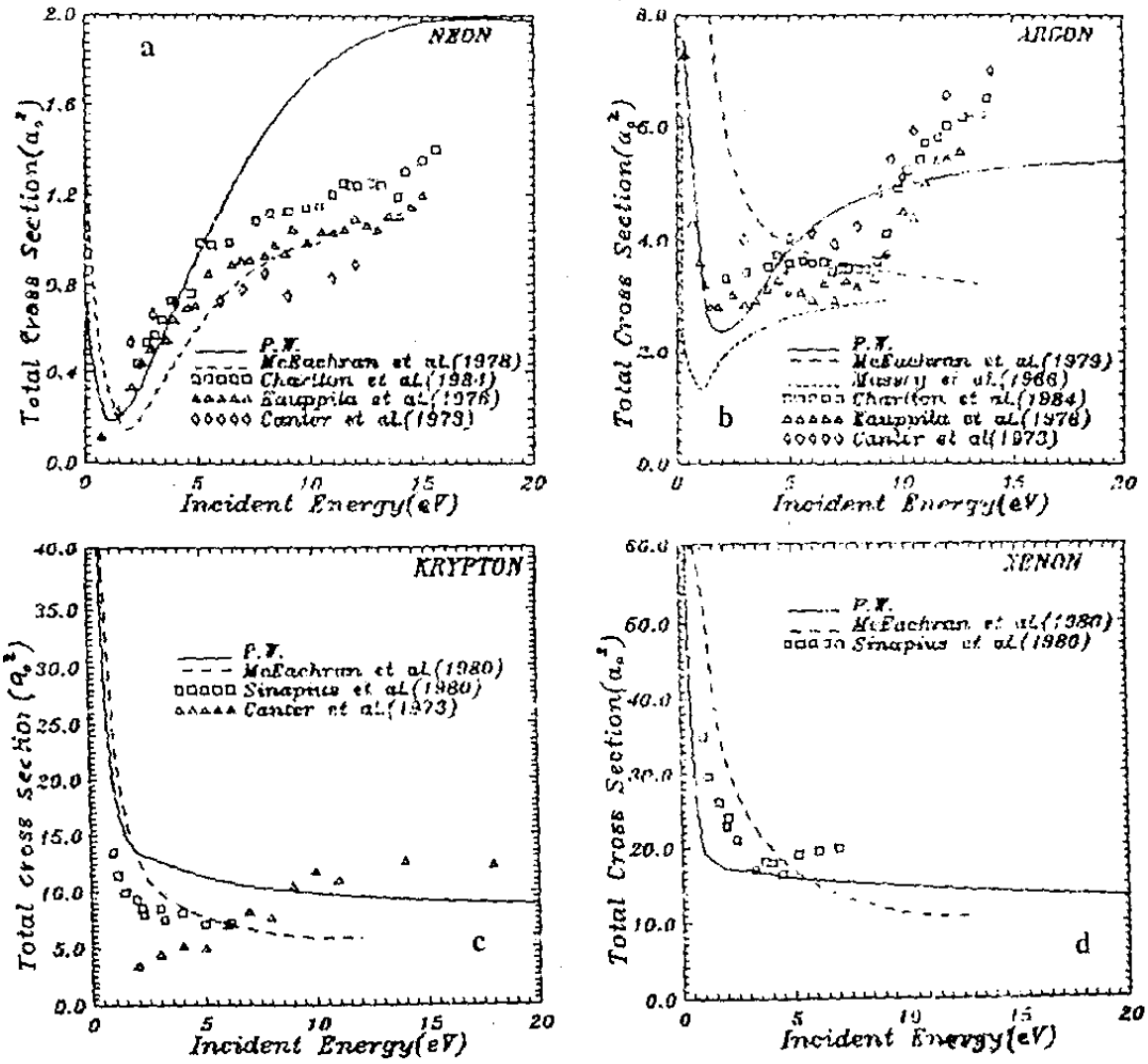


**Fig. 9:** Total cross-sections (in $a_o^2$) for positron scattering from inert gases atoms.

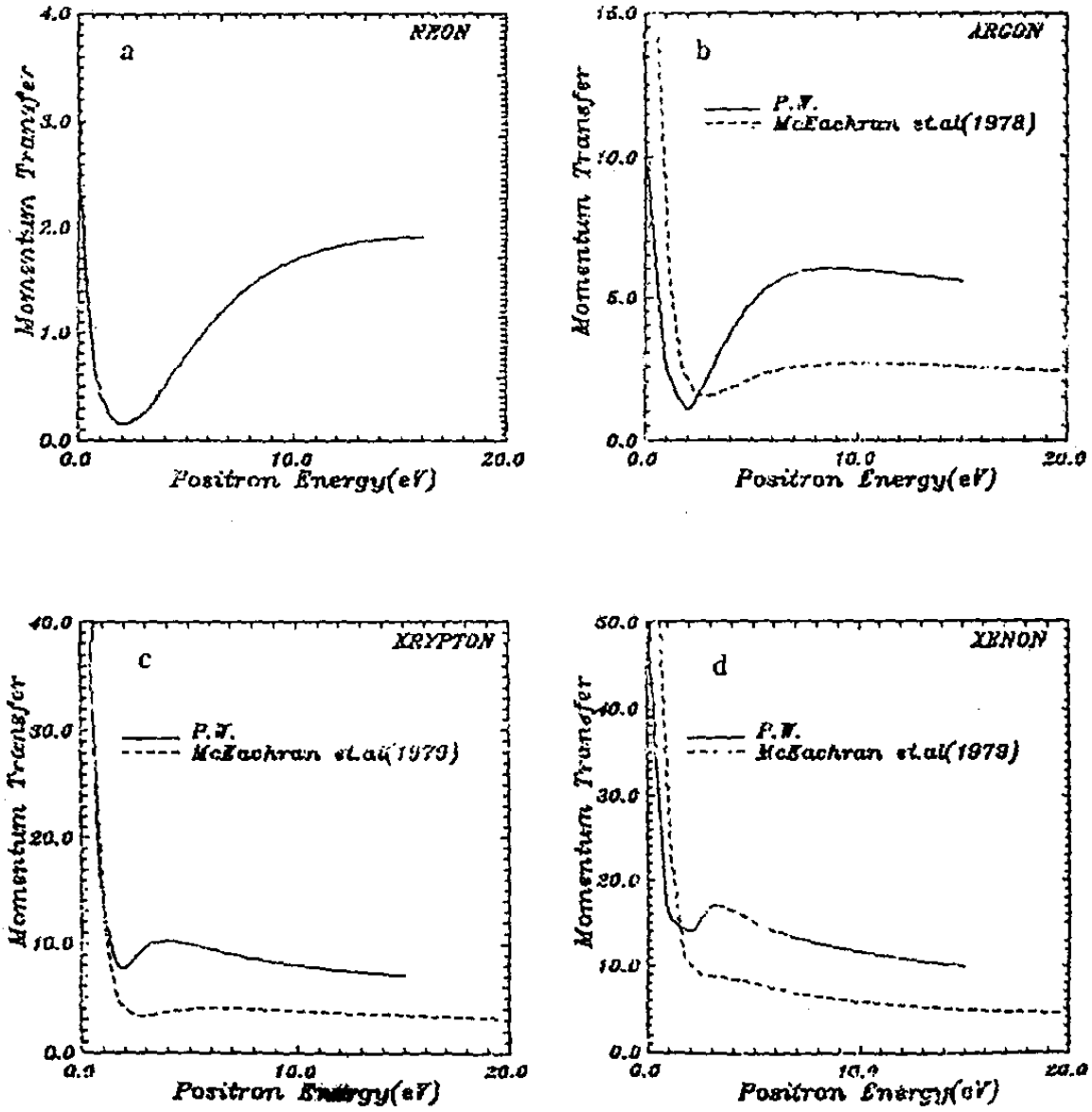


**Fig. 10:** Momentum transfer cross sections for positron scattering from inert gases atoms.

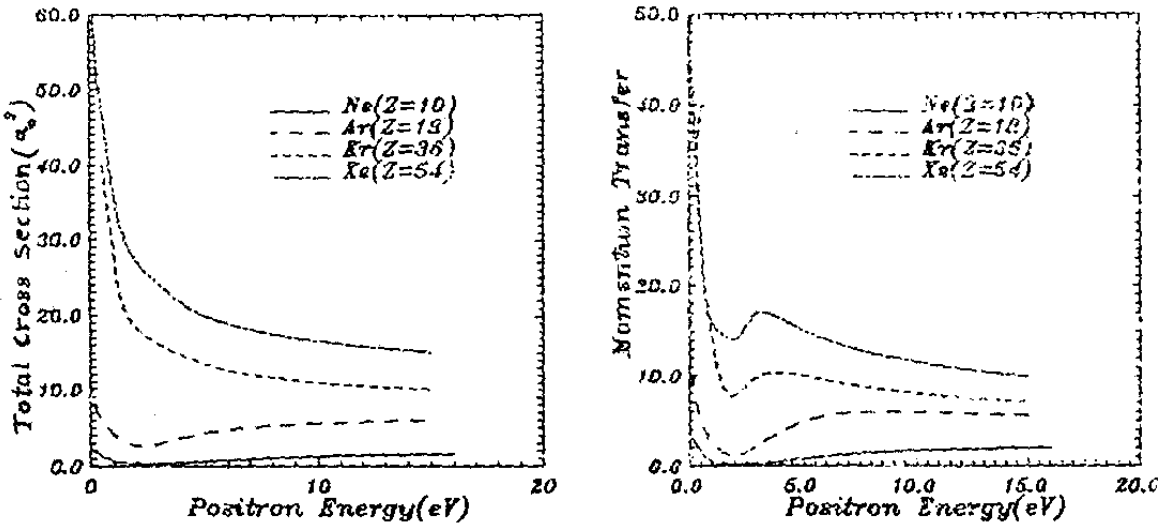


**Fig. 11:** Total (Ramsaure maximum) and Momentum transfer (Townsend maximum) cross-sections for positron scattering from inert gases atoms

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## الاستطارة المرنة للبوزترونات من ذرات الغازات الخاملة عند الطاقات الواطئة و المتوسطة باستخدام جهد استقطاب متعدد الحدود

**علاء عبد الحسن خلف و فلحي عبد الحسن علي**

***قسم الفيزياء / كلية العلوم / جامعة البصرة / البصرة / العراق***

***المستخلص :***

تم حساب ازاحات الطور و المقاطع العرضية التفاضلية ( DCS's ) و المقاطع العرضية الكلية ( TCS's ) و المقاطع العرضية للزخم المنتقل ( MTCS's ) للبوزترونات عند الطاقات الواطئة و المتوسطة لذرات الغازات الخاملة ( النيون ، الاركون ، الكربتون و الزينون ) .

اعتمدت هذه الطريقة النظرية على ربط الجهد المستقر ( الاستاتيكي ) مع جهد الاستقطاب الثنائي و الرباعي عند المسافات الطويلة ومع الجهد الترابطي للباحث Ashok Jain . عند المسافات القصيرة وجدنا ان هناك توافق جيد لنتائجنا مع النتائج العملية و النظرية المتوفرة لباحثين اخرين .