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Elastic scattering of electrons by krypton and the free–free absorption coefficient of Kr^-

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Abstract. Elastic scattering of electrons by krypton atoms is considered using the R-matrix method. Phaseshifts, differential, integral and momentum transfer cross sections are reported for electron impact energies in the range 0.01-16 eV.

The free-free absorption coefficient of the negative ion of krypton is also calculated for wavelengths longer than 1500 Å and for a wide range of temperatures.

1. Introduction

For almost two decades, the scattering of low-energy electrons by krypton atoms has received considerable theoretical and experimental study. A wealth of data has been produced for total elastic and momentum transfer cross sections, differential cross sections and phaseshifts. However, considerable disagreement still exists between different sets of experimental data, between different theoretical treatments and between theory and experiment.

In this paper we restrict our attention to the impact energy range 0-16 eV; in this range the two most interesting features in total elastic and momentum transfer cross sections appear, namely the Ramsauer-Townsend minimum and the maximum in the cross sections. Particular attention is paid to the phaseshifts since we also wish to obtain accurate free-free absorption coefficient data for the negative ion of krypton.

The two most recent theoretical calculations in this energy range for the elastic scattering of electrons are those of McEachran and Stauffer (1984) and Fon *et al* (1984). McEachran and Stauffer employed a polarised-orbital approximation which included the dipole part of the polarisation potential as well as exchange potential. However, they did not include polarisation-exchange terms which arise naturally in their theory and which could be of significance at these low energies. Fon *et al* employed an R-matrix approach in which polarisation and exchange were included by coupling a ^1P pseudostate to the krypton ground state. The value of the static polarisability employed in their calculation, 19.7 au is considerably larger than that found by experiment, 16.76 au (Orcutt and Cole 1967) and may account for, at least in part, differences found with experimental data, particularly at the lowest impact energies.

The absorption coefficient for the free-free process

$$e^- + h\nu + Kr \rightarrow e^- + Kr \tag{1}$$

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has been treated theoretically by Geltman (1973), John (1975a, b) and Stallcop (1974). Geltman performed the first sophisticated calculation for process (1). He evaluated the relevant dipole matrix elements using wavefunctions obtained from solutions of the Schrödinger equation in which the electron-atom interaction is represented by a central-field potential. For the potential he employed a Hartree-Fock-Slater potential together with a three-parameter analytical potential selected to yield the correct behaviour ($\sim r^{-4}$) at large electron-atom separations r. The two remaining parameters were obtained by adjusting them to fit the elastic scattering and momentum transfer cross section data available at that time. John (1975a, b) used the 'asymptotic' method proposed by Dalgarno and Lane (1966) in which the absorption coefficient is expressed in terms of the momentum transfer cross section. A modification of this method had been employed earlier by Stallcop (1974) and again experimental values for the momentum transfer cross section were employed.

In this paper we present the first *ab initio* calculation of the free-free absorption coefficient using sophisticated electron-krypton scattering wavefunctions in evaluating, without further approximation, the relevant matrix elements for a wide range of wavelengths and temperatures.

2. Theory

In this paper an R-matrix approach is adopted and the calculations are performed using the R-matrix program described by Berrington *et al* (1978). We assume that the effects of spin-orbit coupling and other relativistic effects may be neglected and that the calculation may be performed in LS coupling. The calculation of Sin Fai Lam (1982) would support the neglect of relativistic effects. Two states of krypton were included in the eigenfunction expansion. The ground state of krypton was represented by the single-configuration Hartree-Fock wavefunction obtained by Clementi and Roetti (1974). A ^{1}P pseudostate was added to this (to allow for the ground-state static dipole polarisability) and this ^{1}P state was represented by a linear combination of four configurations, namely

$$a_1(4s4p^6\overline{5p}) + a_2(4s^24p^5\overline{5s}) + a_3(4s^24p^5\overline{5d}) + a_4(4s^24p^5\overline{4d}) \tag{2}$$

where

$$a_1 = -0.070\,279 \qquad a_2 = 0.585\,711 \qquad a_3 = 0.501\,888 \qquad a_4 = -0.632\,544$$

and in (2) all subshells not specified are closed.

For both atomic states the one-electron radial orbitals are expressed in the form

$$P_{nl}(r) = \sum_i c_i r^{p_i} \exp(-\zeta_i r) \tag{3}$$

and for the ns, $n = 1$-4; np, $n = 2$-4; nd, $n = 3$ orbitals the parameters c_i, p_i and ζ_i were taken from Clementi and Roetti (1974). The parameters for the other orbitals are given in table 1. Those for 4d were determined by optimising the ground-state energy by including the three configurations arising from $4p^4\overline{4d}^2$ together with the closed shell ground-state configuration, using the program CIV3 (Hibbert 1975). The remaining orbitals were determined by requiring that the ^{1}P^o pseudostate together with the single configuration ground state gave for the ground-state static polarisability the value of 16.787 au, this value being in agreement with that obtained by the more sophisticated calculation of Hibbert *et al* (1987) and in close accord with the experimental value of

Table 1. Values of parameters for the pseudo-orbitals.

Orbital	c_i	p_i	ζ_i
$\overline{4d}$	129.951 46	3	7.425 66
	−4.604 35	4	2.280 62
$\overline{5s}$	8.780 57	1	24.051 59
	−101.052 02	2	14.233 37
	100.024 12	3	7.191 73
	−14.270 39	4	3.432 15
	0.156 87	5	1.406 16
$\overline{5p}$	175.868 65	2	15.967 70
	−170.906 62	3	7.115 47
	22.044 38	4	3.166 86
	−0.980 53	5	1.927 16
$\overline{5d}$	1.194 49	3	1.368 90
	−1.705 14	4	1.368 90
	0.471 51	5	1.368 90

16.763 au (Orcutt and Cole 1967). We note that the present representation of the pseudostate differs from that used by Fon *et al* (1984) firstly by the omission of a 4f pseudo-orbital so that the 3d shell remains closed in the present calculation and secondly by providing a superior value of the dipole polarisability.

The R-matrix program was then utilised by including 16 continuum orbitals for each incident electron orbital angular momentum $l = 0, 1, 2, 3$ and 4, the R-matrix radius being taken to be 12.6 au. Limitations on the number of $(N+1)$-electron correlation configurations were imposed in order to make the calculation tractable; for the symmetries considered, namely $^2S^e$, $^2P^o$, $^2D^e$ and $^2F^o$ all configurations arising from $4s4p^6$ or $4s^24p^5$ plus two electrons distributed in all possible ways among 4s, 4p, $\overline{4d}$, $\overline{5s}$, $\overline{5p}$ and $\overline{5d}$ orbitals were included; for the $^2S^e$ and $^2P^o$ symmetries additional configurations were allowed by considering $4s4p^5$ plus three electrons distributed among the 4s, 4p, $\overline{5s}$, $\overline{5p}$ and $\overline{5d}$ orbitals. For these lowest symmetries the additional flexibility was found to be essential in order to obtain sensible results. All of the cross section data presented in the next section were obtained as described and where necessary higher partial-wave contributions were added by employing phaseshifts derived from the effective-range theory of Rosenberg *et al* (1961)—in the energy range under consideration these corrections are quite small.

Finally, we consider the free-free process (1). For the case in which the krypton atom is in its ground state both initially and finally, the R-matrix multichannel theory (Bell *et al* 1977) gives for the free-free absorption coefficient (including stimulated emission):

$$K_\lambda(T) = 4.655\times10^{-17}T^{-5/2}\lambda^{-1}[1-\exp(-1.439\times10^8 T^{-1}\lambda^{-1})]$$
$$\times\sum_{l_i l_f}\sum_{L_i L_f}\int \mathrm{d}(k_i^2)|\langle\psi_f^-\|M\|\psi_i^+\rangle|^2\exp(-1.579\times10^5 T^{-1}k_i^2) \qquad \mathrm{cm^4\,dyn^{-1}}$$

where T denotes the temperature (K), λ the photon wavelength (Å), i and f the initial and final states of the system, l and L the angular momenta of the free electron and the total system respectively and k the radial momentum of the free electrons. The electron–atom elastic scattering functions ψ are determined using the R-matrix theory

described above. Calculations have been performed using the dipole-length formulation for the operator M and in the summations over angular momenta we include transitions $S \leftrightarrow P$, $P \leftrightarrow D$ and $D \leftrightarrow F$.

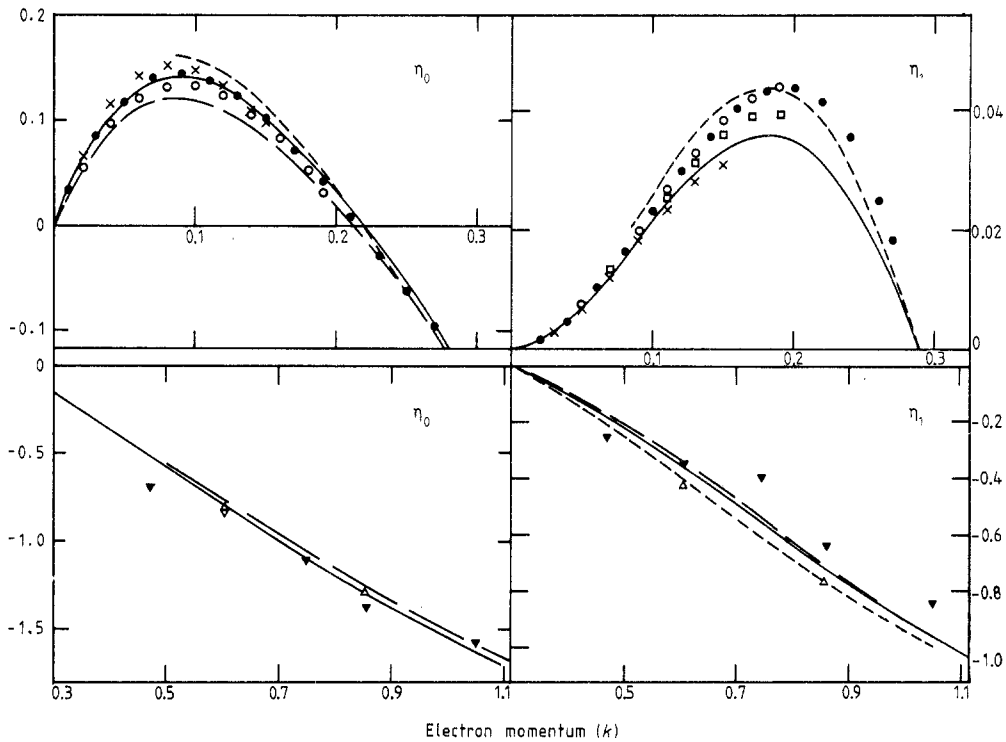
3. Results and discussion

3.1. Phaseshifts

The present values for the phaseshifts η_l, $l = 0, 1, 2, 3$ are given in table 2 and are compared with other theoretical values and with experimentally derived data in figures 1(*a*) and 1(*b*). For clarity the $l = 0$ data of Fon *et al* (1984) for $k \geq 0.3$ and the $l = 1$ data of McEachran and Stauffer (1984) for $k \leq 0.3$ are not shown and in both cases the data agree with the present values. For η_0 and η_1 and $k \geq 0.3$, the theoretical data are in satisfactory accord within the different approximations used and with experiment although further and more accurate experimental data in this energy region are clearly desirable. For $k \leq 0.3$ and η_0, the present results are in better agreement with experiment than the data of Fon *et al* (1984) and McEachran and Stauffer (1984), particularly in the region of the maximum in η_0. The results for η_1 for $k \leq 0.3$ show more diversity;

Table 2. Total elastic (Q) and momentum transfer (Q_M) cross sections (in units of πa_0^2) and phaseshifts (η) (rad) for the elastic scattering of electrons by krypton. Superscripts denote the power of ten by which the number is to be multiplied.

E (eV)	Q	Q_M	η_0	η_1	η_2	η_3
0.01	3.34^{1}	3.14^{1}	7.83^{-2}	2.41^{-3}	3.89^{-4}	1.31^{-4}
0.04	2.09^{1}	1.82^{1}	1.23^{-1}	7.99^{-3}	1.39^{-3}	4.58^{-4}
0.08	1.36^{1}	1.08^{1}	1.39^{-1}	1.44^{-2}	2.90^{-3}	9.51^{-4}
0.1	1.13^{1}	8.55	1.41^{-1}	1.72^{-2}	3.65^{-3}	1.21^{-3}
0.2	5.20	3.03	1.29^{-1}	2.74^{-2}	7.53^{-3}	2.46^{-3}
0.3	2.68	1.10	1.04^{-1}	3.31^{-2}	1.15^{-2}	3.70^{-3}
0.4	1.46	3.64^{-1}	7.44^{-2}	3.54^{-2}	1.56^{-2}	4.94^{-3}
0.5	8.80^{-1}	1.29^{-1}	4.45^{-2}	3.53^{-2}	1.99^{-2}	6.17^{-3}
0.6	6.35^{-1}	1.28^{-1}	1.49^{-2}	3.31^{-2}	2.43^{-2}	7.44^{-3}
0.7	5.95^{-1}	2.49^{-1}	-1.42^{-2}	2.92^{-2}	2.88^{-2}	8.73^{-3}
0.8	6.85^{-1}	4.32^{-1}	-4.25^{-2}	2.40^{-2}	3.32^{-2}	1.00^{-2}
0.9	8.66^{-1}	6.54^{-1}	-7.00^{-2}	1.78^{-2}	3.80^{-2}	1.13^{-2}
1.0	1.11	8.99^{-1}	-9.67^{-2}	1.08^{-2}	4.28^{-2}	1.27^{-2}
2.0	4.81	3.78	-3.27^{-1}	-8.10^{-2}	9.77^{-2}	2.60^{-2}
3.0	8.90	7.09	-5.11^{-1}	-1.81^{-1}	1.68^{-1}	3.84^{-2}
4.0	1.29^{1}	1.07^{1}	-6.67^{-1}	-2.76^{-1}	2.54^{-1}	5.05^{-2}
5.0	1.68^{1}	1.42^{1}	-8.02^{-1}	-3.64^{-1}	3.56^{-1}	6.31^{-2}
6.0	2.06^{1}	1.73^{1}	-9.22^{-1}	-4.46^{-1}	4.68^{-1}	7.69^{-2}
7.0	2.40^{1}	1.96^{1}	−1.03	-5.22^{-1}	5.85^{-1}	9.15^{-2}
8.0	2.69^{1}	2.09^{1}	−1.13	-5.92^{-1}	7.03^{-1}	1.07^{-1}
9.0	2.89^{1}	2.12^{1}	−1.22	-6.57^{-1}	8.14^{-1}	1.23^{-1}
10.0	3.02^{1}	2.06^{1}	−1.30	-7.17^{-1}	9.15^{-1}	1.41^{-1}
11.0	3.07^{1}	1.96^{1}	−1.37	-7.72^{-1}	1.00	1.60^{-1}
12.0	3.07^{1}	1.82^{1}	−1.45	-8.24^{-1}	1.08	1.80^{-1}
13.0	3.03^{1}	1.68^{1}	−1.51	-8.71^{-1}	1.14	2.02^{-1}
14.0	2.96^{1}	1.55^{1}	−1.58	-9.11^{-1}	1.19	2.26^{-1}
15.0	2.90^{1}	1.42^{1}	−1.64	-9.55^{-1}	1.23	2.54^{-1}
16.0	2.85^{1}	1.30^{1}	−1.69	-9.97^{-1}	1.27	2.91^{-1}



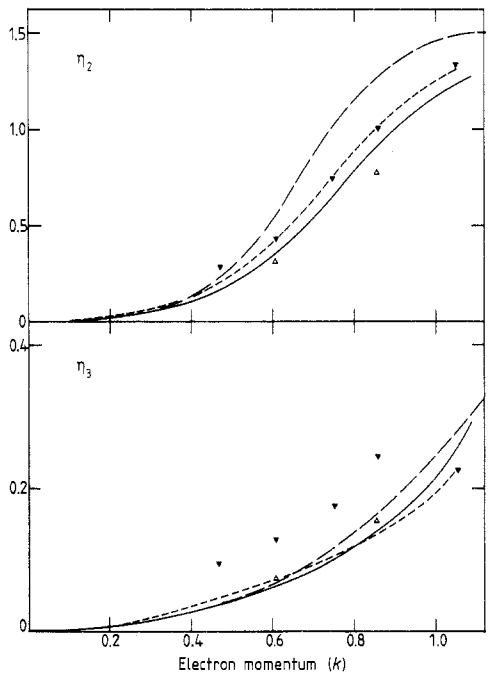


Figure 1. Phaseshifts η_0 and η_1 plotted against electron momentum k (au). Theoretical values: ——, present results - - -, Fon *et al* (1984); — —, McEachran and Stauffer (1984); △, Haberland *et al* (1986). Experimental data: ▼, Srivastava *et al* (1981); ×, Guskov *et al* (1978); ○, Buckman and Lohmann (1987); ●, Weyhreter *et al* (1988) ($E_{max} = 1.0$ eV); □, Weyhreter *et al* (1988) ($E_{max} = 0.5$ eV).

the present values are in excellent accord with those of McEachran and Stauffer (1984) and with experiment at the lowest impact energies but both sets of data have a maximum lower than the experimental derived values. The maximum in η_1 clearly requires further investigation since the data of Guskov *et al* (1978) would suggest a maximum lower than that found by the other experimentalists—Buckman and Lohman (1987) and Weyrheter *et al* (1988); note that the $l=1$ phaseshift derived by Weyrheter *et al* (1988) from their differential cross section measurements using effective range theory differs at the maximum when this theory is applied to an energy range 0–0.5 eV as opposed to 0–1.0 eV (for $l=0$ their results for $E_{max}=1.0$ eV and $E_{max}=0.5$ eV are almost identical).

The results for η_2 and η_3 displayed in figure 1(*b*) show that considerable uncertainty still remains for these phaseshifts. The greatest uncertainty is for η_2 and the present values lie considerably below those of McEachran and Stauffer (1984) and Fon *et al* (1984) as was also found by Haberland *et al* (1986) from their application of a Kohn–Sham-type one-particle theory to the present problem.

3.2. Differential cross sections

Differential cross sections derived from the present phaseshifts are compared with other theoretical values and with experimental data in figures 2 and 3. For an electron energy of 10 eV, differences between the theoretical results and between experimental values clearly exist. The most recent experimental data of Jost and Otto (1986) lie closest to the theoretical results of McEachran and Stauffer (1984) for scattering angles less than 60° but, in agreement with the present values, the Jost and Otto data do not have a minimum around 70° as found by McEachran and Stauffer. For 5 eV electrons and scattering angles less than 120° the present results are in exceptional accord with both the experimental data of Srivastava *et al* (1981) and with the data of Heindorff *et al* (1976) which we have normalised to those of Srivastava *et al* at 90°. At angles greater than 120°, the present results and those of Haberland *et al* (1986) are in excellent agreement but lie below all other theoretical and experimental data. At 3 eV, the double minimum found by others is again produced by the present work but the first minimum is found to be deeper and to lie at a lower value of the scattering angle. The present results are in excellent agreement with the experimental data of Heindorff *et al* (1976) which we have again normalised to those of Srivastava *et al* (1981) at 90°. At 1 eV, the present differential cross section is in excellent agreement with the experimental data of Weyrheter *et al* (1988) and for scattering angles less than 70° with the theoretical values of McEachran and Stauffer (1984).

Figure 3 compares theoretical differential cross sections with the experimental data of Weyhreter *et al* (1988) for three scattering angles as a function of electron energy over the region of the Ramsauer–Townsend minimum. At a scattering angle of 90°, the present values are in exceptional accord with experiment over the whole energy region—indeed for energies less than 0.4 eV and greater than 0.6 eV the difference is less than 10%. For 60°, similar behaviour and agreement is found although the minimum found experimentally occurs at a higher scattering angle than that presently determined—nevertheless for energies less than 0.45 eV and greater than 1.2 eV the difference is better than 20%. At 30°, agreement is less good, the present results showing a more pronounced minimum and lying considerably higher than experiment for the larger impact energies. Referring to figure 1(*a*), the minimum at 30° in the differential cross section occurs in the energy region where the $l=1$ phaseshift is

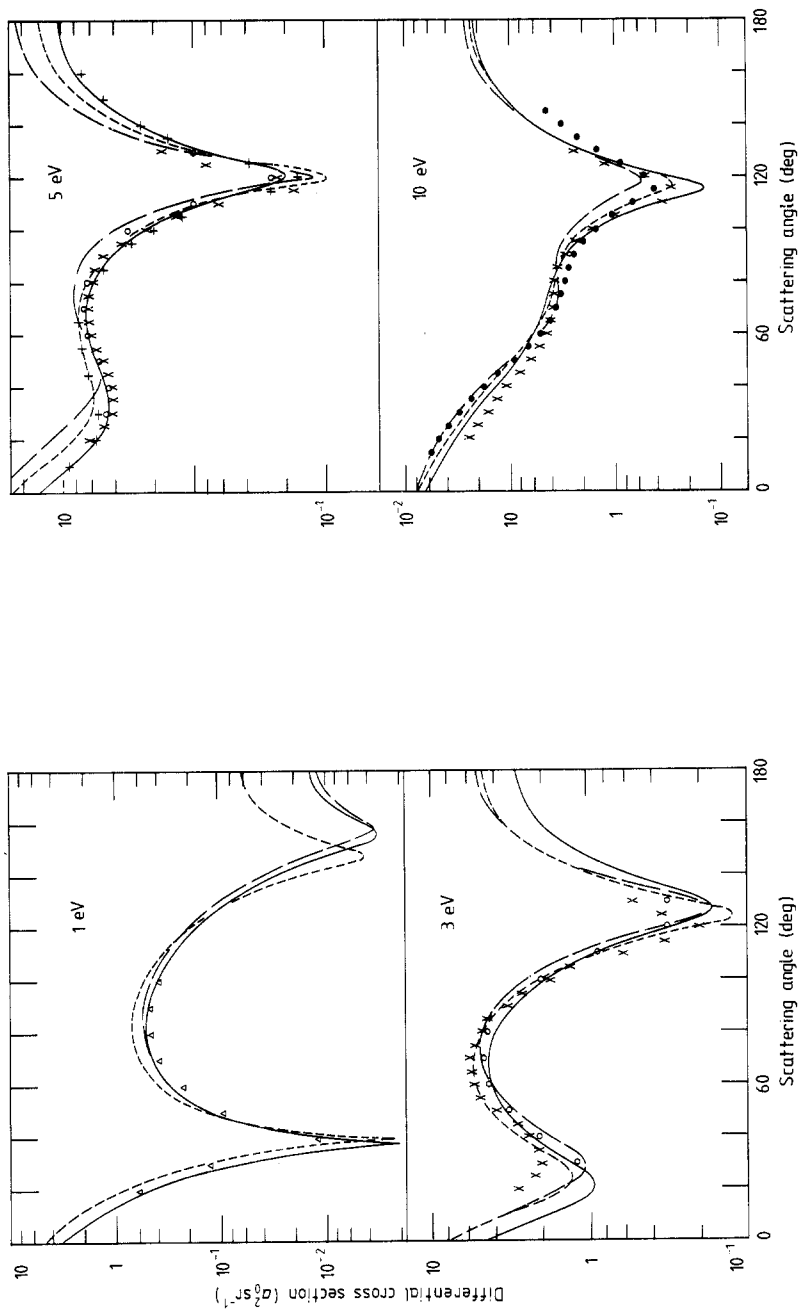


Figure 2. Differential cross sections for elastic scattering of 1, 3, 5 and 10 eV electrons by krypton. Theory: ——, present results; - - -, Fon *et al* (1984); — —, McEachran and Stauffer (1984); +, Haberland *et al* (1986). Experiment: △, Weyhreter *et al* (1988); ●, Jost and Otto (1986); ×, Srivastava *et al* (1981); ○, Heindorff *et al* (1976) (normalised at 90° to the data of Srivastava *et al*).

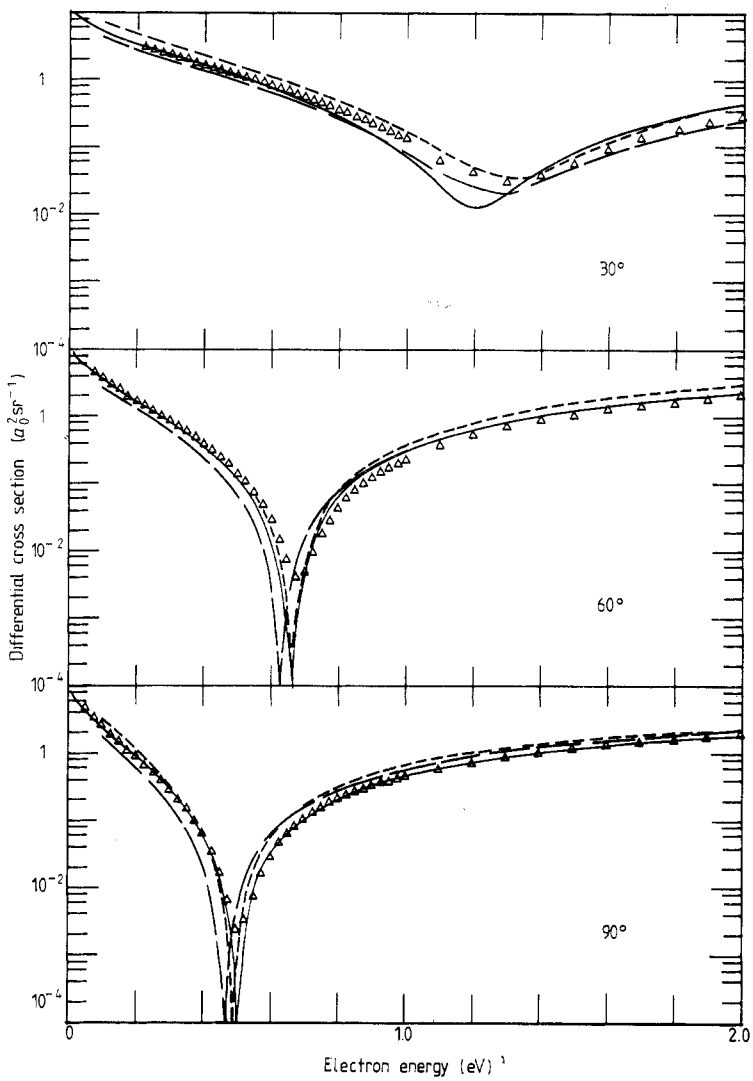


Figure 3. Differential cross sections for elastic scattering at scattering angles 30°, 60° and 90° by electrons from krypton in the energy range 0–2 eV. Theory: ——, present results; - - -, Fon *et al* (1984); — —, McEachran and Stauffer (1984). Experiment: △, Weyhreter *et al* (1988).

passing through zero and hence is sensitive to values for this phaseshift in this region. However the low-energy results are again in excellent accord with experiment, the difference being less than 10% for energies less than 0.5 eV.

3.3. Total cross sections

The present values for the total elastic scattering cross section are given in table 2 and are compared with other theoretical results and with experiment in figure 4. The experimental data of Weyhreter *et al* (1988) have been derived from their equation (6) using the values obtained by them for the effective range coefficients with the

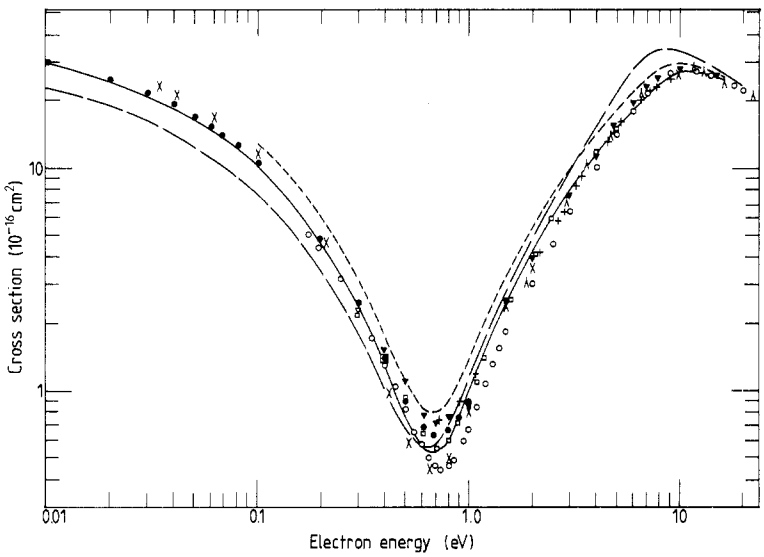


Figure 4. Elastic scattering cross section. Theory: ——, present results; - - -, Fon *et al* (1984); — —, McEachran and Stauffer (1984). Experiment: ●, Weyhreter *et al* (1988); ×, Guskov *et al* (1978); +, Subramanian and Kumar (1987); ○, Buckman and Lohmann (1987); ▼, Jost *et al* (1983); □, Ferch *et al* (1987); ⊥, Dababneh *et al* (1980).

impact-energy upper limit of 1.0 eV. At energies below that at which the Ramsauer-Townsend minimum occurs, the present values are in excellent agreement with the experimental data of Weyhreter *et al* (1988), Buckman and Lohman (1987) and Ferch *et al* (1987), but lie somewhat below that of Guskov *et al* (1978) at the lower impact energies. At energies above that at which the Ramsauer-Townsend minimum occurs, the present results lie closest to, but somewhat above, the experimental data except at the maximum in the cross section where the agreement is excellent. In the neighbourhood of the Ramsauer-Townsend minimum, the present values, unfortunately, provide no means of identification or classification as to which of the many experiments might be most accurate; this is clearly an energy region which requires further investigation.

Table 2 contains present values for the momentum transfer cross section and comparison is made with other data in figure 5. The experimental data of Weyhreter *et al* (1988) have been derived from their equation (7) using the values obtained by them for the effective range coefficients with the impact energy upper limit of 1.0 eV. The present results are in excellent accord with the Weyhreter *et al* data for energies less than 0.4 eV but lie above all other experimental data at the lowest energies. The depth of the Ramsauer-Townsend minimum agrees well with that found by Koizumi *et al* (1986) although its position is displaced to a somewhat higher energy, whilst at higher impact energies the present results lie below previous theoretical values and below the data of Koizumi *et al.* Clearly, further experimental investigation of both the low- and high-energy regions is desirable.

3.4. Free-free absorption coefficient

The present results for the free-free absorption coefficient of the negative ion of krypton are given in table 3 for wavelengths greater than 1500 Å and for a range of temperatures

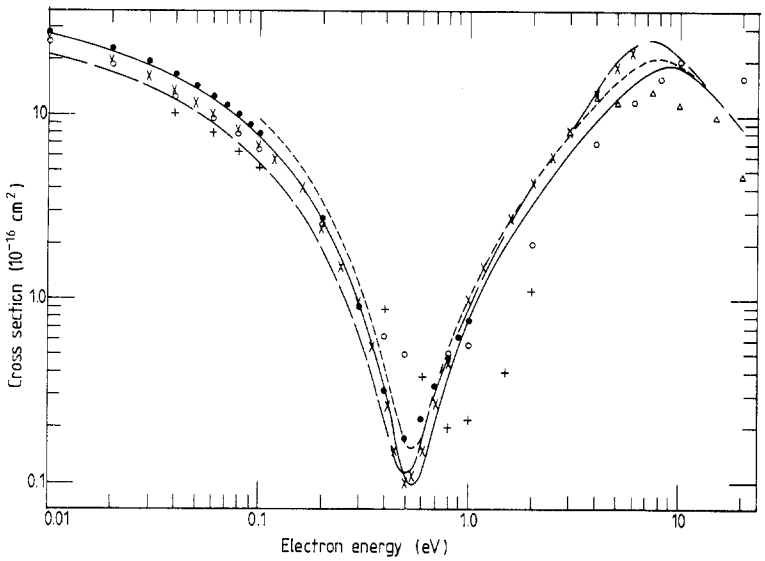


Figure 5. Momentum transfer cross section. Theory: ——, present results; - - -, Fon *et al* (1984); — —, McEachran and Stauffer (1984). Experiment: ●, Weyhreter *et al* (1988); ×, Koizumi *et al* (1986); ○, Frost and Phelps (1964); +, Hoffmann and Skarsgard (1969); △, Srivastava *et al* (1981).

Table 3. Kr^- free-free absorption coefficient (in units of 10^{-26} cm^4 dyn^{-1}). $\theta = 5040/T$. Superscripts denote the powers of ten by which the numbers are to be multiplied.

λ (Å) \ θ	0.5	0.6	0.8	1.0	1.2	1.4	1.6	1.8	2.0	2.8	3.6
151 890	2.17^{1}	1.84^{1}	1.37^{1}	1.07^{1}	8.92	7.89	7.44	7.48	7.90	1.26^{1}	2.05^{1}
113 918	1.22^{1}	1.03^{1}	7.70	6.06	5.04	4.45	4.20	4.21	4.44	6.99	1.13^{1}
91 134	7.83	6.63	4.95	3.89	3.24	2.86	2.70	2.70	2.84	4.42	7.09
45 567	1.98	1.68	1.26	1.00	8.33^{-1}	7.30^{-1}	6.74^{-1}	6.55^{-1}	6.65^{-1}	9.01^{-1}	1.33
30 378	8.95^{-1}	7.66^{-1}	5.82^{-1}	4.64^{-1}	3.87^{-1}	3.36^{-1}	3.04^{-1}	2.86^{-1}	2.79^{-1}	3.22^{-1}	4.29^{-1}
22 784	5.17^{-1}	4.46^{-1}	3.44^{-1}	2.79^{-1}	2.35^{-1}	2.04^{-1}	1.83^{-1}	1.69^{-1}	1.61^{-1}	1.60^{-1}	1.88^{-1}
18 227	3.43^{-1}	2.98^{-1}	2.35^{-1}	1.93^{-1}	1.64^{-1}	1.44^{-1}	1.29^{-1}	1.18^{-1}	1.10^{-1}	9.59^{-2}	9.85^{-2}
15 189	2.50^{-1}	2.20^{-1}	1.76^{-1}	1.48^{-1}	1.28^{-1}	1.13^{-1}	1.03^{-1}	9.43^{-2}	8.78^{-2}	7.36^{-2}	6.93^{-2}
13 019	1.92^{-1}	1.71^{-1}	1.40^{-1}	1.20^{-1}	1.06^{-1}	9.57^{-2}	8.79^{-2}	8.17^{-2}	7.69^{-2}	6.53^{-2}	6.03^{-2}
11 392	1.54^{-1}	1.39^{-1}	1.17^{-1}	1.02^{-1}	9.18^{-2}	8.42^{-2}	7.84^{-2}	7.38^{-2}	7.01^{-2}	6.10^{-2}	5.66^{-2}
10 126	1.28^{-1}	1.17^{-1}	1.00^{-1}	8.96^{-2}	8.19^{-2}	7.62^{-2}	7.18^{-2}	6.83^{-2}	6.55^{-2}	5.84^{-2}	5.47^{-2}
9 113	1.09^{-1}	1.01^{-1}	8.86^{-2}	8.05^{-2}	7.48^{-2}	7.05^{-2}	6.72^{-2}	6.46^{-2}	6.25^{-2}	5.71^{-2}	5.42^{-2}
7 595	8.58^{-2}	8.10^{-2}	7.39^{-2}	6.91^{-2}	6.58^{-2}	6.35^{-2}	6.17^{-2}	6.05^{-2}	5.95^{-2}	5.74^{-2}	5.67^{-2}
6 510	7.08^{-2}	6.82^{-2}	6.43^{-2}	6.18^{-2}	6.01^{-2}	5.91^{-2}	5.85^{-2}	5.81^{-2}	5.80^{-2}	5.84^{-2}	5.97^{-2}
5 696	6.13^{-2}	6.01^{-2}	5.81^{-2}	5.70^{-2}	5.64^{-2}	5.62^{-2}	5.63^{-2}	5.65^{-2}	5.69^{-2}	5.92^{-2}	6.20^{-2}
5 063	5.42^{-2}	5.39^{-2}	5.34^{-2}	5.33^{-2}	5.36^{-2}	5.40^{-2}	5.46^{-2}	5.54^{-2}	5.62^{-2}	5.98^{-2}	6.37^{-2}
4 557	4.89^{-2}	4.93^{-2}	4.99^{-2}	5.06^{-2}	5.14^{-2}	5.23^{-2}	5.33^{-2}	5.43^{-2}	5.53^{-2}	5.97^{-2}	6.43^{-2}
3 645	3.98^{-2}	4.12^{-2}	4.35^{-2}	4.54^{-2}	4.71^{-2}	4.88^{-2}	5.04^{-2}	5.20^{-2}	5.35^{-2}	5.93^{-2}	6.50^{-2}
3 038	3.36^{-2}	3.56^{-2}	3.87^{-2}	4.13^{-2}	4.36^{-2}	4.57^{-2}	4.77^{-2}	4.96^{-2}	5.15^{-2}	5.84^{-2}	6.51^{-2}
2 604	2.88^{-2}	3.10^{-2}	3.46^{-2}	3.76^{-2}	4.01^{-2}	4.25^{-2}	4.46^{-2}	4.67^{-2}	4.86^{-2}	5.59^{-2}	6.28^{-2}
2 278	2.48^{-2}	2.71^{-2}	3.09^{-2}	3.40^{-2}	3.67^{-2}	3.91^{-2}	4.14^{-2}	4.35^{-2}	4.55^{-2}	5.29^{-2}	5.99^{-2}
1 823	1.82^{-2}	2.04^{-2}	2.41^{-2}	2.72^{-2}	2.98^{-2}	3.22^{-2}	3.45^{-2}	3.65^{-2}	3.86^{-2}	4.60^{-2}	5.30^{-2}
1 519	1.27^{-2}	1.45^{-2}	1.77^{-2}	2.04^{-2}	2.29^{-2}	2.51^{-2}	2.72^{-2}	2.92^{-2}	3.11^{-2}	3.83^{-2}	4.51^{-2}

$0.5 \leqslant \theta \leqslant 3.6$ where $\theta = 5040/T$. An interesting feature of these results is that, at the longer wavelengths, the absorption coefficient for a given wavelength displays a minimum as a function of θ. This minimum is closely related to the Ramsauer-Townsend minimum and arises from the different angular momenta transitions contributing to the coefficient. Table 4 illustrates in more detail how such a minimum arises together with an indication of the relative importance of individual contributions to the total absorption coefficient. For both wavelengths the P↔D and D↔F contributions are monotonically decreasing as θ increases and for small values the P↔D contribution is the dominant one; for $\lambda = 9113$ Å the S↔P contribution is relatively constant but for $\lambda = 91\,134$ Å a minimum is clearly present and for large θ this contribution dominates.

Table 5 compares the present results with earlier calculations. The 'asymptotic' approximation values of John (1975a, b) and Stallcop (1974) are similar and for all temperatures and long wavelengths both agree to within 30-40% with the present results; however for the shorter wavelengths the approximation clearly fails, the difference rising to factors of 2 or 3. Similar behaviour exists for the comparison with

Table 4. Contributions to the absorption coefficient from various transitions at wavelengths 91 134 and 9113 Å (in units of 10^{-26} cm^4 dyn^{-1}).

L_i \ θ / L_L	$\lambda = 91\,134$ Å					$\lambda = 9\,113$ Å				
	0.5	1.0	1.6	2.0	2.8	0.5	1.0	1.6	2.0	2.8
S→P	0.94	0.90	1.17	1.67	3.38	0.008	0.007	0.006	0.005	0.004
P→S	1.07	0.94	0.68	0.58	0.58	0.020	0.026	0.027	0.027	0.027
Subtotal	2.01	1.84	1.85	2.25	3.96	0.028	0.033	0.033	0.032	0.031
P→D	2.45	0.87	0.33	0.22	0.20	0.059	0.042	0.032	0.029	0.025
D→P	2.13	0.71	0.24	0.15	0.10	0.013	0.004	0.002	0.001	0.001
Subtotal	4.58	1.58	0.57	0.37	0.30	0.072	0.046	0.034	0.030	0.026
D→F	0.64	0.25	0.15	0.13	0.10	0.005	0.001	0.000	0.000	0.000
F→D	0.60	0.22	0.12	0.10	0.07	0.004	0.001	0.000	0.000	0.000
Subtotal	1.24	0.47	0.27	0.23	0.17	0.009	0.002	0.000	0.000	0.000
Total	7.83	3.89	2.70	2.84	4.42	0.109	0.081	0.067	0.062	0.057

Table 5. Kr^- free-free absorption coefficient: ratio of present results to other theoretical values. G, Geltman (1973); J, John (1975a, b); S, Stallcop (1974).

	T(K)								
	2500			5000			10 000		
λ(μm)	G	J	S	G	J	S	G	J	S
0.5	1.48	1.75	—	1.29	3.27	—	1.19	2.76	—
1.0	1.17	0.70	—	1.03	1.72	—	1.02	1.65	—
2.0	0.70	0.46	—	0.84	1.29	—	0.94	1.38	1.36
5.0	0.57	0.65	—	0.78	1.29	1.39	0.91	1.30	1.30
10.0	0.57	0.84	0.95	0.78	1.32	1.37	0.91	1.28	1.29
15.0	0.57	0.93	0.95	0.78	1.36	1.37	0.91	1.28	1.29
20.0	0.57	0.93	0.95	0.77	1.35	1.36	0.91	1.28	1.29

the results of Geltman (1973) except that for the lowest temperature and all wavelengths considerable disagreement exists.

The accuracy of the present results is difficult to assess and must await further calculations of even more sophistication. However we believe that they are the most accurate currently available particularly at long wavelengths and high values of θ since our very low-energy phaseshifts are seen to be in exceptionally good agreement with experiment.

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