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Alpha particle and deuteron impact L-shell ionization of Ar, Cu, Ge, Br, Zr and Ag

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Abstract. Alpha particle and deuteron impact L-subshell ionization cross-sections of Ar, Cu, Ge, Br, Zr and Ag have been computed using Vriens' expressions for ionization cross-section of atoms due to impact of heavy charged particles. The effects of Coulomb deflection of the projectile and increase in binding of the target electron in the presence of projectile have been incorporated. Hartree-Fock velocity distributions for the target electrons have been used in the present calculations. The simple binary encounter approximation model is found to give results which are in satisfactory agreement with those obtained from experiments and from other theories.

Keywords. Alpha particle; deuteron impact; L-shell ionization.

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1. Introduction

Theoretical studies of ion-impact inner shell ionization of atoms are of much relevance as they can be used to obtain cross-sections for emission of x-rays from various inner shells which have wide applications (Hardt and Watson 1976; Starter *et al* 1981). Further, these studies provide a means for testing the various theories of direct ionization. Among all the inner shells the L-shell is particularly important for this purpose because it consists of three subshells having different properties e.g. shape of wave function. Moreover, it has been studied more extensively as compared to other higher shells and therefore detailed experimental and theoretical results are available for comparison (Bearse *et al* 1973; Gray *et al* 1975).

The binary encounter approximation (BEA) has been successfully used for theoretical calculations of ion impact inner-shell ionization cross-sections of atoms (Garcia 1970; Kumar and Roy 1978; Langenberg 1978; Chatterjee *et al* 1983; Shrivastava *et al* 1984; Shrivastava and Roy 1986). In fact the BEA, apart from its simplicity, is essentially linked with the plane wave Born approximation (PWBA) and gives results which are in agreement with the PWBA, semiclassical approximation (SCA) and the available experimental results (Gray *et al* 1975; Chatterjee *et al* 1983). For refinement of theoretical results several corrections e.g. Coulomb deflection of the projectile in the field of the target nucleus, increase in binding of the target electron in the presence of projectile, polarization of the orbital of the target electron, relativistic effects for the target electron (Brandt and Lapicki 1979) and energy loss effect (Brandt and Lapicki 1981) have been proposed. In a previous paper (Chatterjee *et al* 1983) we have reported our BEA results for proton impact L-shell ionization cross-sections for some atoms incorporating the corrections for the first two effects mentioned above and obtained good agreement with experiments and other theoretical calculations. In the present work we have studied the L-shell ionization of Ar, Cu, Ge, Br, Zr and Ag due to impact of deuterons and alpha particles in the energy range 50–2000 keV incorporating the corrections for the first two effects mentioned earlier following the BEA method of Garcia (1970) and the perturbed stationary state (PSS) method suggested by Brandt and Lapicki (1979), respectively. Other effects are not expected to be important in the energy range considered and for the targets studied in this work. In order to test the utility of the procedure adopted for incorporating binding energy correction we have calculated the ratio of alpha to deuteron-induced ionization cross-sections because this ratio is insensitive to other factors (Jesus *et al* 1983). The present work will also enable us to investigate the effect of electronic wave function on the inner shell ionization cross-sections.

2. Method of calculation

Vriens' expressions (1967) for ionization cross-sections of atoms due to impact of heavy charged particles incorporating the modifications for the effects of Coulomb repulsion of the projectile and increase in binding of the target electron can be written as

$$Q = \begin{cases} \dfrac{(s+s')^2}{s^2 s'^2 U_c^2} Z_1^2 \left(1 + \dfrac{2t^2}{3} - \dfrac{1}{4(s'^2 - t^2)}\right)(\pi a_0^2), & 1 \leq 4s'(s'-t) \\ \dfrac{(s+s')^2}{2s^2 s'^2 U_c^2 t} Z_1^2 \left[\dfrac{1}{4(s'+t)} + t + \tfrac{2}{3}\{2s'^3 + t^3 - (1+t^2)^{3/2}\}\right](\pi a_0^2), & \\ 0 & 4s'(s'-t) \leq 1 \leq 4s'(s'+t) \\ & 1 \geq 4s'(s'+t), \end{cases} \qquad (1)$$

where $t^2 = v_{2L}^2/U_c, \quad s^2 = v_1^2/U_c,$

$s'^2 = s^2 - (1{\cdot}058 Z_1 Z_{2L})/(1836 M a_{2L} U_c)$, Z_1 and M

are the charge and mass of the projectile, a_{2L} is the radius of the shell considered, $Z_{2L} = Z_2 - s_{2L}$ with Z_2 equal to the nuclear charge of the target and s_{2L} the screening constant of the shell. In equation (1) $U_c = \varepsilon U_{2L}$ is the binding energy of the target electron corrected for the presence of the projectile inside the shell, where U_{2L} is the unperturbed binding energy of the target electron and $\varepsilon = 1 + (2/Z_{2L}\theta_{2L})g$ with

$$\theta_{2L} = 4U_{2L}/(Z_{2L}^2 \times 13{\cdot}6),$$

$$g = (1 + 9X + 31X^2 + 49X^3 + 162X^4 + 63X^5 + 18X^6 + 1{\cdot}97X^7)/(1+X)^9 \quad \text{for } L_{\text{I}} \text{ subshell}$$

and

$$g = (1 + 10X + 45X^2 + 102X^3 + 331X^4 + 6{\cdot}7X^5 + 58X^6 + 7{\cdot}8X^7 + 0{\cdot}888X^8)/(1+X)^{10} \quad \text{for } L_{\text{II}} \text{ and } L_{\text{III}} \text{ subshells}$$

and $X = v_1/\frac{1}{2}\theta_{2L}v_{2L}$ (Brandt and Lapicki 1979; Chatterjee *et al* 1983). In the above expressions all quantities have been expressed in atomic units with energy in rydbergs (Kumar and Roy 1978). Cross-sections have been obtained by integrating the above expressions over the Hartree-Fock momentum distribution for the target electron constructed using the Hartree-Fock radial functions given by Clementi and Roetti (1974). The binding energies of the target electrons and the quantum mechanical values of screening constants have been taken from Lotz (1968) and Fisher (1972) respectively. For subshell radii of atoms the quantum-mechanical values of points of maximum radial probability density reported by Desclaux (1973) have been used.

3. Results and discussion

In order to compare our results with experimental x-ray production cross-sections we have converted (except in case of Ar) our subshell ionization cross-section (σ_L) into subshell x-ray production cross-section (σ_{LX}) using the relation $\sigma_{LX} = \omega_L \sigma_L$, where ω_L is the subshell fluorescence yield. In the present work theoretical values of fluorescence yield reported by Bambynek *et al* (1972) have been used.

In case of Ar (see figure 1) L_I-subshell ionization cross-sections have been computed

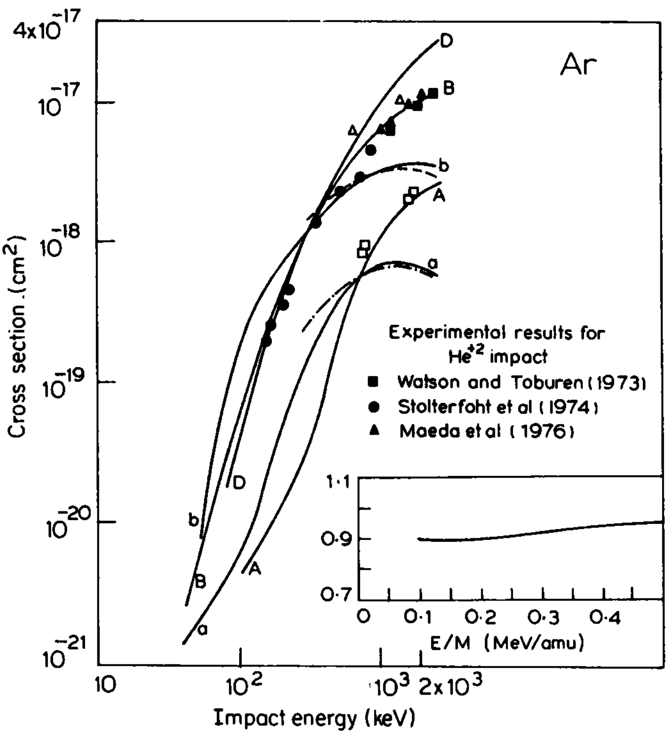

Figure 1. Ionization cross-sections for Ar. (i) Alpha particle impact cross-sections: Curves A and B: Present values of σ_{L_I} and σ_L respectively; Curve D: σ_L by Brandt and Lapicki (1979). △ and □: σ_L and σ_{L_I} respectively by Choi (1978). (ii) Deuteron impact cross-sections: Curves a and b: Quantities corresponding to curves A and B -·- σ_{L_I} by Choi (1978) --- σ_L by Choi (1978).

separately while those of L_{II} and L_{III} subshells jointly using the mean of the ionization energies and radii of L_{II} and L_{III} subshells and treating all the six electrons in the $2p$ shell equivalent. This approach seems to be justified as the difference in the binding energies of L_{II} and L_{III} subshells is only 2·1 eV (Lotz 1968). The present results for α-particle impact are in better agreement with the more recent experimental cross-sections. Our results are slightly larger than those of Stolterfoht *et al* (1974) which might be due to the fact that the latter results are in the low energy region where the BEA is not suitable. The present calculations also show close agreement with the CPSSR (Coulomb) perturbed stationary state including relativistic effects) results of Brandt and Lapicki (1979) in case of α-particle impact and Hartree-Slater calculations of Choi (1978) in case of deuteron and α-particle impact both. Our calculated values of the ratio $\sigma_\alpha/4\sigma_d$ rise rapidly with E/M (MeV/amu) at first but the variation becomes much slower for higher values of E/M. The L_I-subshell ionization cross-section curves (a and A) show inflection which is a general feature for this subshell (Gray *et al* 1975; Langenberg 1978; Chen *et al* 1982). The inflection shifts towards higher impact energy in case of alpha particle impact.

Cross-sections for Cu, Ge, Br, Zr and Ag have been presented in figures 2–6. The calculated cross-sections for Zr and Ag are in close agreement with the recent

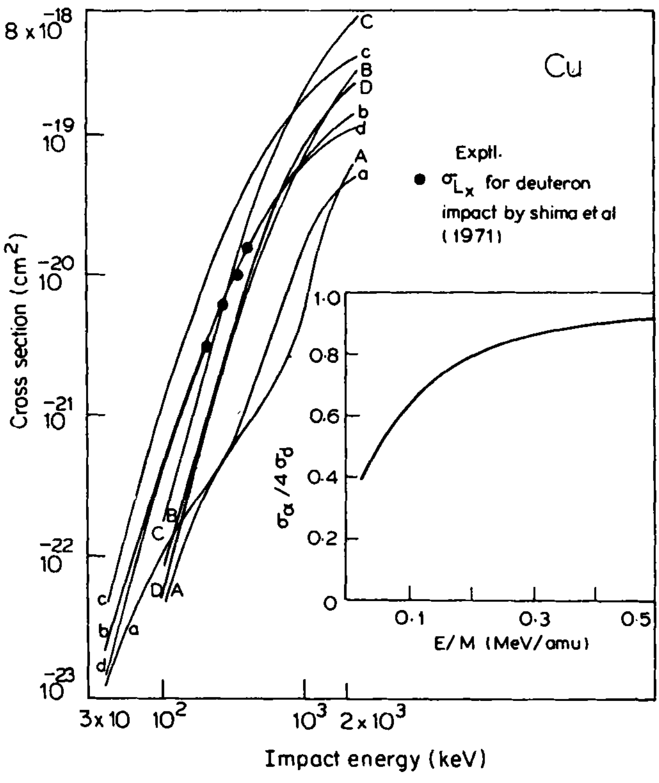

Figure 2. Cross-sections of Cu. Curves A and a: Same as in figure 1; Curves B and C: Present values of $\sigma_{L_I}+\sigma_{L_{II}}$ and σ_L respectively; Curve D: $10^2\times\sigma_{LX}$ (present values); Curves b, c and d: Quantities (deuteron impact) corresponding to curves B, C, D.

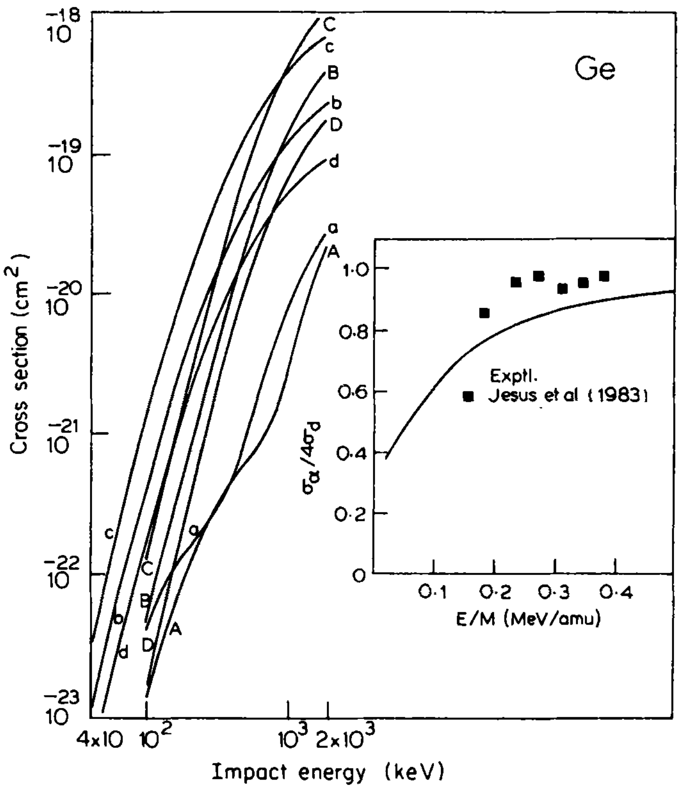

Figure 3. Cross-sections for Ge. Same as in figure 2 except Curves D and d: $10 \times \sigma_{LX}$ for He^{2+} and deuteron impact respectively (present results).

experimental measurements reported by Jesus *et al* (1983) both for alpha particle and deuteron projectiles. Our deuteron impact cross-sections in case of Cu and Ag are in good agreement with the experimental observations of Shima *et al* (1971). The present values of the ratio $\sigma_\alpha/4\sigma_d$, in case of Br, Zr and Ag are close to the experimental ratios of Jesus *et al* (1983) as regards the magnitude and nature of variation with E/M. In case of Ge the experimental values of $\sigma_\alpha/4\sigma_d$ show a slight structure which has not been observed in our calculations.

4. Conclusion

From a close inspection of figures 1–6 we conclude that the present method gives a good account of L-shell ionization of atoms due to impact of alpha particles and deuterons in the energy range investigated. It is observed that the L_{II} and L_{III} subshell ionization cross-sections show a smooth variation with incident energy but the L_I subshell ionization cross-section curve shows an inflection which becomes more and more pronounced and shifts towards higher impact energy with increase in atomic number of the target and the charge and mass of the projectile. Further, L_I subshell ionization cross-sections are found to be higher than those for L_{II} subshell in the low energy range

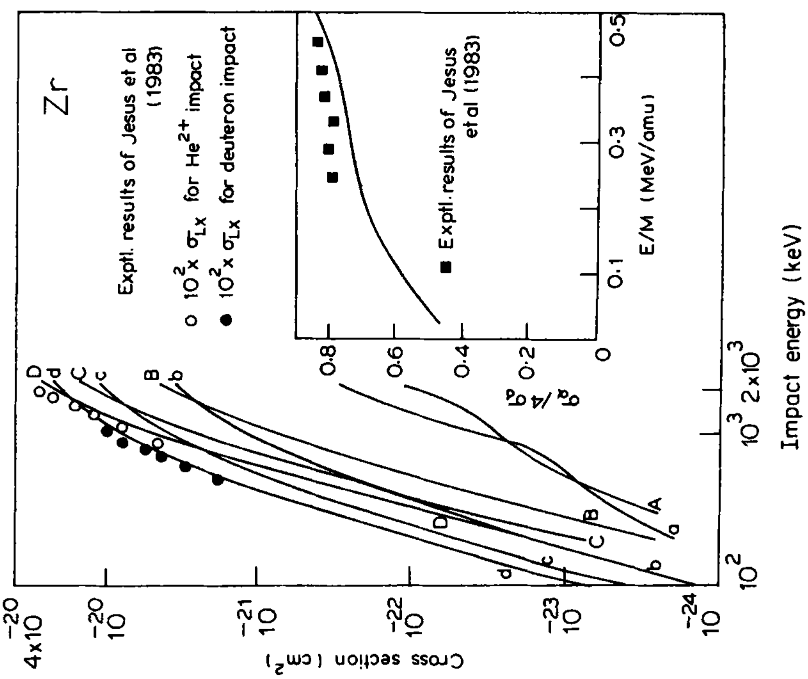

Figure 5. Cross-sections for Zr. Same as in figure 2.

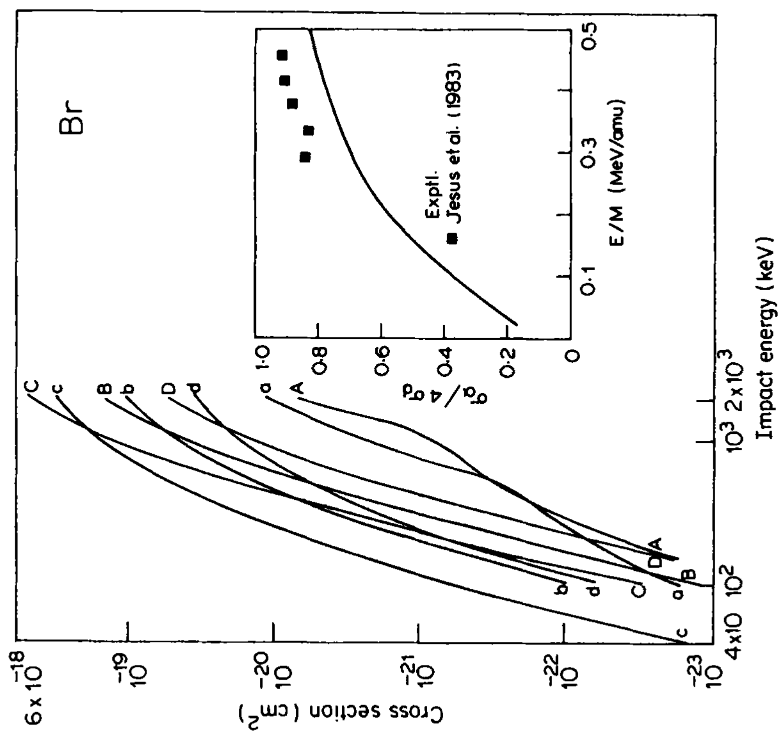

Figure 4. Cross-sections for Br. Same as in figure 3.

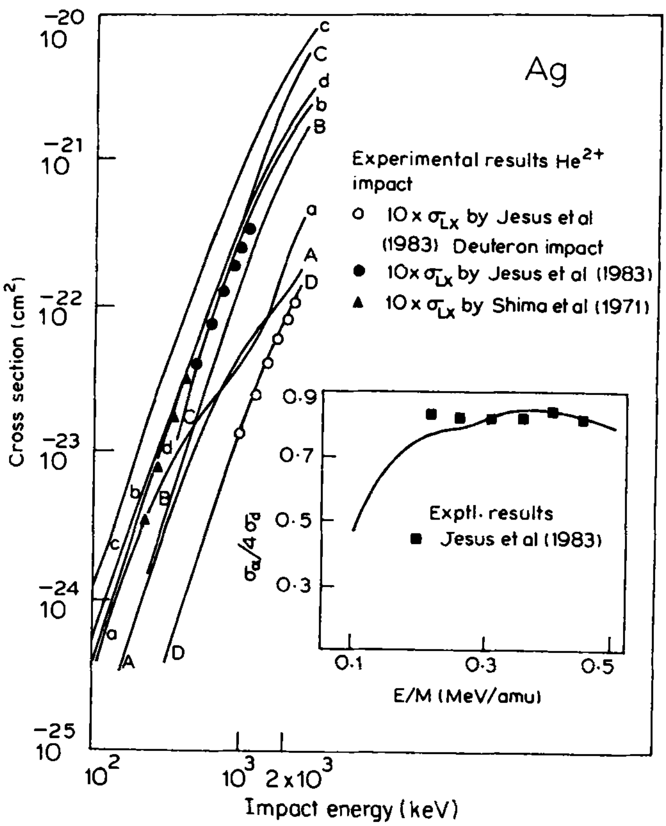

Figure 6. Cross-sections for Ag. Same as in figure 3.

although the binding energy of the former is higher than that for the latter. These features have been attributed to the extra node in the 2*s* radial wave function as compared to 2*p*-wave function (Gray *et al* 1975; Langenberg 1978; Chen *et al* 1982; Jitschin *et al* 1982). The close agreement between the calculated and experimental values of the ratio $\sigma_\alpha/4\sigma_d$ suggests that the binding energy correction factor suggested by Brandt and Lapicki (1979) works well with the BEA calculations also.

We would now like to briefly discuss the kinematic and Coulombic effects of the projectile on the ionization cross-sections. The unmodified expressions for the ionization cross-sections show that at a fixed projectile velocity the ionization cross-section is proportional to the square of the projectile charge but independent of projectile mass, so that $\sigma_d/\sigma_p = 1$ whereas $\sigma_\alpha/\sigma_p = 4$ (σ_p = proton impact *L*-shell ionization cross-section). However, comparing our proton impact *L*-shell ionization cross-sections (including the modifications) reported earlier (Chatterjee *et al* 1983) with the present results we find that $\sigma_d/\sigma_p > 1$ and approaches 1·0 whereas $\sigma_\alpha/\sigma_p < 4$ and tends to 4 with increase in impact velocity. These findings are in accordance with theoretical considerations. The Coulomb deflection correction increases with increase in the ratio Z_1/M whereas the binding effect depends only on the projectile charge and increases with it. Consequently reduction in cross-section due to Coulomb deflection effect is greater in case of proton impact than in case of deuteron impact but the binding effect is same in both cases. Therefore $\sigma_p/\sigma_d < 1$ at low impact velocities. Further for equivelocity proton and alpha particle, Coulomb deflection effect is greater with the former whereas the binding energy correction is greater in the latter case. As the binding effect dominates over the Coulomb deflection effect there is greater reduction in alpha particle impact ionization cross-sections due to the combined effect. Therefore $\sigma_\alpha/\sigma_p < 4$ at low incident velocities.

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References

Bambynek W, Craseman B, Fink R W, Freund H U, Mark H, Swift C D, Price R E and Rao P V 1972 *Rev. Mod. Phys.* **44** 786
Bearse R C, Close D A, Malanify J J and Umberger C J 1973 *Phys. Rev.* **A7** 1269
Brandt W and Lapicki G 1979 *Phys. Rev.* **A20** 465
Brandt W and Lapicki G 1981 *Phys. Rev.* **A23** 1717
Chatterjee S N, Kumar A and Roy B N 1983 *Physica* **C122** 275
Chen M H, Crasemann B and Mark H 1982 *Phys. Rev.* **A26** 1243
Choi B H 1978 *Phys. Rev.* **A11** 2004
Clementi E and Roetti C 1974 *At. Data Nucl. Data Tables* **14**
Desclaux J P 1973 *At. Data Nucl. Data Tables* **12** 325
Fischer C F 1972 *At. Data Nucl. Data Tables* **4** 301
Garcia J D 1970 *Phys. Rev.* **A1** 280
Gray T J, Light G M, Gardner R K and McDaniel F D 1975 *Phys. Rev.* **A12** 2393
Hardt T L and Watson R L 1976 *Phys. Rev.* **A14** 137
Jesus A P, Pimental I R and Lopes J S 1983 *Nucl. Instrum. Methods* **214** 29
Jitschin W, Kaschuba A, Hippler R and Lutz H O 1982 *J. Phys.* **B15** 763
Kumar A and Roy B N 1978 *J. Phys.* **B11** 1435
Langenberg A 1978 Ph.D. Thesis, Phys. Lab. Rijksuniversiteit, Utrecht
Lotz W 1968 *J. Opt. Soc. Am.* **58** 236
Maeda N, Kobayashi N, Hori H and Sakisaka M 1976 *J. Phys. Soc. Jpn* **40** 1430
Shima K, Makino I and Sakisaka M 1971 *J. Phys. Soc. Jpn* **30** 611
Shrivastava S K, Kumar A and Roy B N 1984 *Physica* **C124** 127
Shrivastava S K and Roy B N 1986 *Physica* **C138** 219
Starter W, Mommsen H, Sarkar M, Schurkes P and Weller A 1981 *J. Phys.* **B14** 2843
Stolterfoht N, Schneider D and Ziem P 1974 *Phys. Rev.* **A10** 81
Vriens L 1967 *Proc. Phys. Soc.* **90** 935
Watson R L and Toburen L H 1973 *Phys. Rev.* **A7** 1953