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ANGULAR DISTRIBUTION OF AUGER ELECTRONS DUE TO 3d-SHELL IMPACT IONIZATION OF KRYPTON

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ABSTRACT

Cross sections for electron impact ionization of krypton due to ejection of a 3d-shell electron have been calculated using screened hydrogenic and Hartree-Slater wave functions for target atom. While the total ionization cross sections in the two approximations are within 10% of each other, the Auger electron angular distribution, related to cross sections for specific magnetic quantum numbers of the 3d electrons, are widely different in the two approximations. The angular distribution due to Hartree-Slater approximation is in excellent agreement with measurement. The physical reason for the discrepancies in the two approximations is explained.

The inner shell vacancies produced by impact ionization of atoms as is well known do not have spacial isotropic distribution. As a result the Auger electrons which follow the vacancy production will also have anisotropic angular distribution (Cleff and Mehlhorn 1974a). The measurement of this angular distribution can thus throw light on the accuracy of different atomic models which have been used to calculate the ionization cross section.

The angular distribution of Auger electrons due to the electron impact L shell ionization of argon has been measured by Cleff and Mehlhorn (1974b) and has been shown to be in satisfactory agreement with the theoretical distribution derived from the calculation of McFarlane (1972).

In a recent experiment Dobelin, Sandner and Mehlhorn (1974) have measured the angular distribution of Auger electrons due to the electron impact M shell ionization of krypton. They have found unsatisfactory agreement between their data and the unpublished screened hydrogenic calculational results of this author. In what follows we present a similar calculation based on Hartree-Slater type wave function for the target atom.

In an ionizing collision between a structureless charged particle and an atom in which an atomic electron is ejected let the initial state of the ejected electron be given by $n\ell m_0$, with n and ℓ the principal and angular momentum quantum numbers, and m_0 the magnetic quantum number with respect to the direction of the incident beam as the Z-axis. If the electron is ejected with an energy ε/Ry, the ionization cross section, $dQ(n\ell m_0)/d(\varepsilon/Ry)$, according to the Born approximation and the central field approximation for the target atom wave function is given by

$$\frac{dQ(n\ell m_0)}{d(\epsilon/Ry)} = \frac{8\pi a_0^2 (M/m_0) Z^2}{E/Ry} \times \int_{a_0(k_1-k_2)}^{a_0(k_1+k_2)} \frac{d(a_0 K)}{(a_0 K)^3} \int \left| \langle \underset{\sim}{k} | e^{i\underset{\sim}{K}\cdot\underset{\sim}{r}} | n\ell m_0 \rangle \right|^2 d\hat{k} \tag{1}$$

where Z is the projectile's charge in units of the absolute value of the electronic charge, E/Ry is the center of mass energy in rydberg, M/m_e is the reduced mass in units of the electron mass, and a_0 is the Bohr radius. $|n\ell m_0\rangle$ and $|\underset{\sim}{k}\rangle$ are the initial and final wave functions of the ejected electron given by

$$|n\ell m_0\rangle = r^{-1} P_{n\ell}(r)\, Y_{\ell m_0}(\hat{r}) \tag{2}$$

$$|\underset{\sim}{k}\rangle = \sum_{\ell'=0}^{\infty} i^{\ell'} \exp(-i\eta_{\ell'})\, r^{-1} P_{\epsilon\ell'}(r) \times \sum_{m'=-\ell'}^{\ell'} \frac{4\pi}{2\ell'+1} Y_{\ell' m'}^{*}(\hat{r})\, Y_{\ell' m'}(\hat{k}) \tag{3}$$

In equations (2) and (3) ℓ' and m' are the final state angular and magnetic quantum numbers of the ejected electron, $Y_{\lambda\mu}(\hat{n})$ are the spherical harmonics corresponding to a unit vector $\hat{n}$, $r^{-1}P_{n\ell}(r)$ and $r^{-1}P_{\varepsilon\ell}(r)$ represent the radial part of the bound and continuum electron wave functions, and $\eta_{\ell'}$ is a phase factor due to the non-coulombic nature of the wave function.

In (1) $\hat{k}$ is a unit vector in the direction of the ejected electron, and k_1 and k_2 are the magnitudes of $\underset{\sim}{k}_1 = \underset{\sim}{p}_1/\hbar$ and $\underset{\sim}{k}_2 = \underset{\sim}{p}_2/\hbar$, where $\underset{\sim}{p}_1$ and $\underset{\sim}{p}_2$ are the center of mass initial and final momenta.

From the conservation of energy we have that

$$a_0 k_1 = (ME/m_e Ry)^{1/2}, \quad a_0 k_2 = [M(E - I - \epsilon)/m_e Ry]^{1/2} \quad (4)$$

with I the ionization potential of the ejected electron. In the derivation of (1) it has been assumed that the initial and final wave functions are orthogonal to each other.

The total ionization cross section is given by

$$Q(n l m_0) = \int_0^{\frac{1}{2}(E-I)} \frac{dQ(n l m_0)}{d\epsilon} \, d\epsilon \quad (5)$$

where the upper limit of the integral is chosen to be ½(E-I) instead of E-I as being given by the conservation of energy. This is according to a prescription given by Peterkop (1961) and this choice compensates to some extent for the fact that the exchange effect is neglected in (1).

To facilitate the evaluation of the matrix in (1) it is convenient to choose the Z-axis along $\underset{\sim}{K}$. If m represents the initial state magnetic quantum number of the ejected electron with respect to $\underset{\sim}{K}$ as the Z-axis, then

$$|n l m_0\rangle = \sum_m d^{\,l}_{m_0 m}(\beta)\, |n l m\rangle \quad (6)$$

where $d^{\ell}_{m_0 m}(\beta)$ are elements of the rotation matrix due to the rotation angle β (Edmonds 1960), and β is given by (McFarlane 1972).

$$\cos\beta = \frac{k_1^2 - k_2^2 + K^2}{2 k_1 K} \quad (7)$$

For evaluation of the integrals in (1) we make use of (6), (2) and (3). We also expand exp $(i\underset{\sim}{K}.\underset{\sim}{r})$ in terms of the spherical harmonics of $\hat{K}$ and $\hat{r}$, and carry out the integration with respect to $\hat{r}$ and $\hat{k}$. Making use of symmetries of $d^{\ell}_{m_o m}(\beta)$ (Edmonds 1960) we obtain

$$\int |\langle \underset{\sim}{k} | e^{i \underset{\sim}{K} \cdot \underset{\sim}{r}} | n \ell m_o \rangle|^2 d\hat{k} = 16\pi^2 (2\ell+1) \sum_{\ell' \lambda} \frac{(2\lambda+1)^2}{2\ell'+1}$$
$$\times \sum_{m=0}^{\ell} \left(1 - \frac{1}{2}\delta(m,0)\right) \left\{ [d^{\ell}_{m_o m}(\beta)]^2 + [d^{\ell}_{m_o m}(\pi-\beta)]^2 \right\}$$
$$\times \left[\begin{pmatrix} \ell & \lambda & \ell' \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} \ell & \lambda & \ell' \\ m & 0 & -m \end{pmatrix} R(\ell\ell'\lambda, kK) \right]^2, \tag{8}$$

$$\ell' = 0, 1, 2, \cdots ; \quad \lambda = |\ell-\ell'|, |\ell-\ell'|+2, \cdots, \ell+\ell', \tag{9}$$

$$R(\ell\ell'\lambda, kK) = \int P_{\epsilon\ell'}(r) \, j_\lambda(Kr) \, P_{n\ell}(r) \, dr \tag{10}$$

A summation with respect to m_o of (8) leads to

$$\sum_{m_o=-\ell}^{\ell} \int |\langle \underset{\sim}{k} | e^{i \underset{\sim}{K} \cdot \underset{\sim}{r}} | n \ell m_o \rangle|^2 d\hat{k}$$
$$= 16\pi^2 (2\ell+1) \sum_{\ell'\lambda} \frac{2\lambda+1}{2\ell'+1} \left[\begin{pmatrix} \ell & \ell' & \lambda \\ 0 & 0 & 0 \end{pmatrix} R(\ell\ell'\lambda, kK) \right]^2 \tag{11}$$

Numerical values of $R(\ell\ell'\lambda, kK)$ are obtained according to the two approximations used. Combination of (8), (1), and (5), and a numerical integration with respect to K and ε will yield the cross section.

In the screened hydrogenic approximation coulomb wave function is used for evaluation of $P_{n\ell}(r)$ and $P_{\varepsilon\ell'}(r)$ occurring in (10). The effective charge for the initial state, Z_{eff}, is obtained from

The total cross section, however, in the two approximations is about the same; in the range 500-3000 eV incident energy the difference between the two values of the total cross section is from 5 to 13%.

Using the calculated values of $\sigma(m_0)$ and formulation of Cleff and Mehlhorn (1974a) the Auger electron angular distribution for transitions $M_4N_{2,3}N_{2,3}(^1S_0)$ and $M_5N_{2,3}N_{2,3}(^1S_0)$ in krypton for two incident energies are calculated and shown in Figures 2 and 3. The agreement between Hartree-Slater approximation and the experimental data is remarkable. An independent calculation by Berezhko and Kabachnic (1975) for the coefficient of anisotropy, using approximation similar to those used here, gives also satisfactory agreement with the experimental data.

The interesting result that emerges from the present calculation is that the use of the Hartree-Slater wave function for the target atom leads to satisfactory agreement between calculation and measurement. The screened hydrogenic wave function gives satisfactory results for the total ionization cross section, but errorneous results for $\sigma(m_0)$. The physical reason for this behavior follows.

The explanation is based on the fact that for large impact parameters the atomic potential can be approximated by a coulomb potential. To show this we assume that the angular momentum state of the target atom during collision is given predominantly by a signle eigenstate, an assumption which is justified for large impact parameters. The electronic density of the target is then almost spherically symmetric.

For a spherically symmetric charge distribution of the target atom the potential seen by the incident electron can be evaluated in the following way. The potential from the electronic cloud within a sphere of a radius equal to the distance of the incident electron from the origin is by the Gass's law coulombic, and is equal to a central coulomb potential whose charge is equal to the charge within the sphere. This charge is equal to -S with S the screening parameter. The potential due to the electronic cloud outside the sphere is non-coulombic.

At high impact energies where the contribution to the cross section comes from large impact parameters the atomic potential is predominantly coulombic. This gives rise to the good agreement obtained between the screened hydrogenic and the Hartree-Slater approximations. For calculation of $\sigma(m_0)$ the atomic potential is not spherically symmetric, thus the discrepancy between the two approximations.

Similarly, for calculating the differential cross section for small scattering angles corresponding to large impact parameters, the atomic potential can be assumed coulombic, and screened hydrogenic should be considered applicable. For large scattering angles with deep atomic potential penetration such approximation does not apply.

Manson's program (Manson 1972) was used to generate R $(2\ell'\lambda, kK)$ according to the Hartree-Slater approximation. The range of ℓ' provided was ℓ'=0-15. This range in the energy range considered is sufficient to give the total cross section to three significant figures. To check the accuracy of the cross section use also has been made of the invariance of the total cross section when $d^{\ell}_{m_0 m}(\beta)$ matrix is replaced by a unit matrix.

In Table 1 several values of $\sigma(m_o)$ for a number of incident energies are given.

I am indebted to S. T. Manson for providing me with his program on Hartree-Slater approximation. Similarly, I gratefully acknowledge the programming help of E. C. Sullivan, and discussions with H. L. Kyle and V. Jacobs.

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Figure Caption

Figure 1. 3d-shell electron impact ionization cross section of krypton, σ, as a function of the incident energy. The curves marked by different values of m_0 give cross sections for ejection of 3d-electrons whose magnetic quantum numbers with respect to the incident beam as the Z-axis are m_0. The curves marked total is the sum of the cross sections with respect to m_0.

Figure 2. Angular distribution of the $M_4N_{2,3}N_{2,3}(^1S_0)$ Auger electrons of krypton. The two theoretical distributions are compared with the experimental data with the error bars of Dobelin et al. (1974). The intensity is normalized to $I(\theta = 90^0) = 1$.

Figure 3. Angular distribution of the $M_5N_{2,3}N_{2,3}$ $(^1S_0)$ of krypton. Notations the same as in Figure 2.

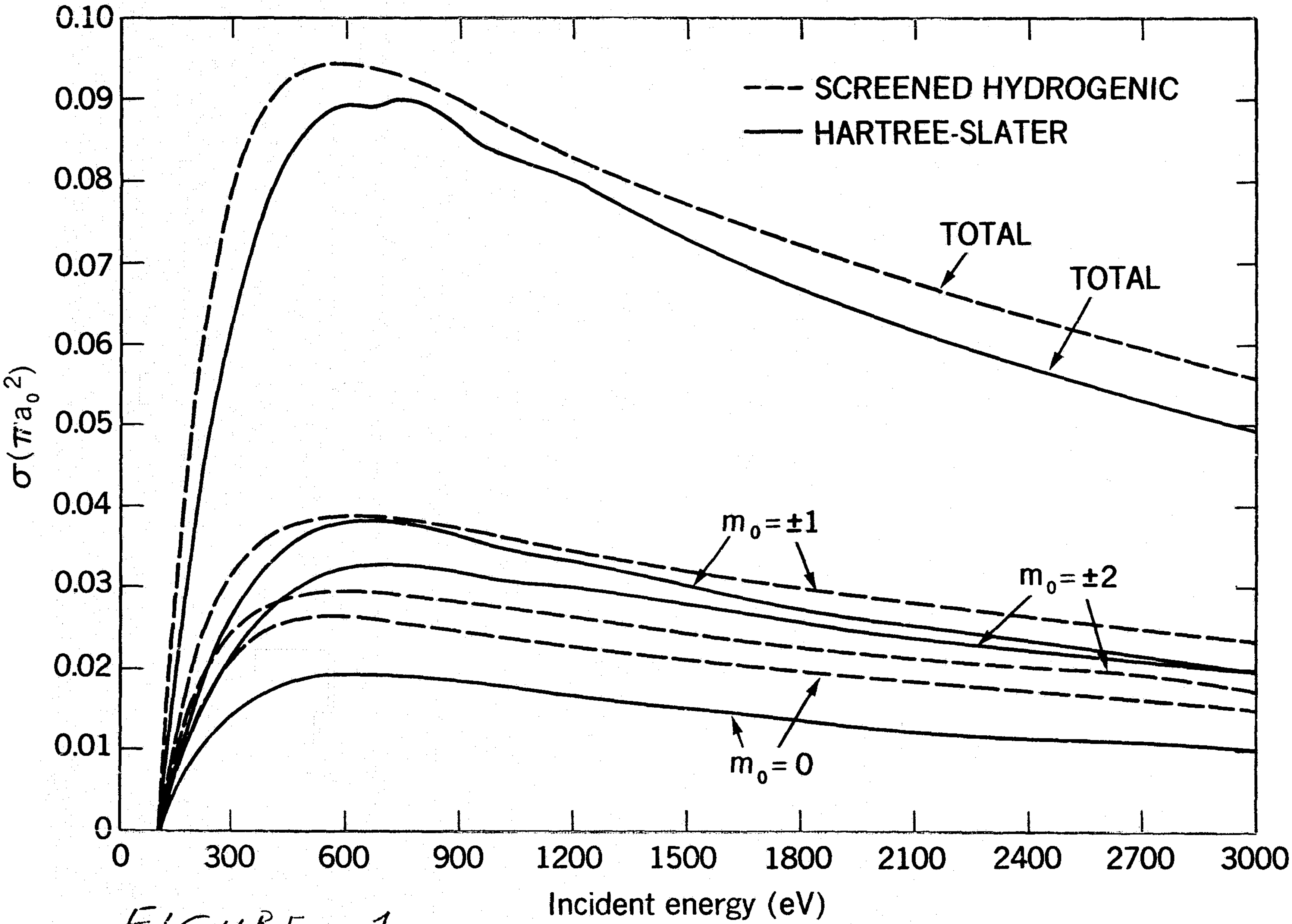
SCREENED HYDROGENIC
HARTREE-SLATER
TOTAL
TOTAL
$m_0 = \pm 1$
$m_0 = \pm 2$
$m_0 = 0$
$\sigma(\pi a_0^2)$
0.10
0.09
0.08
0.07
0.06
0.05
0.04
0.03
0.02
0.01
0
0
300
600
900
1200
1500
1800
2100
2400
2700
3000
Incident energy (eV)

FIGURE 1

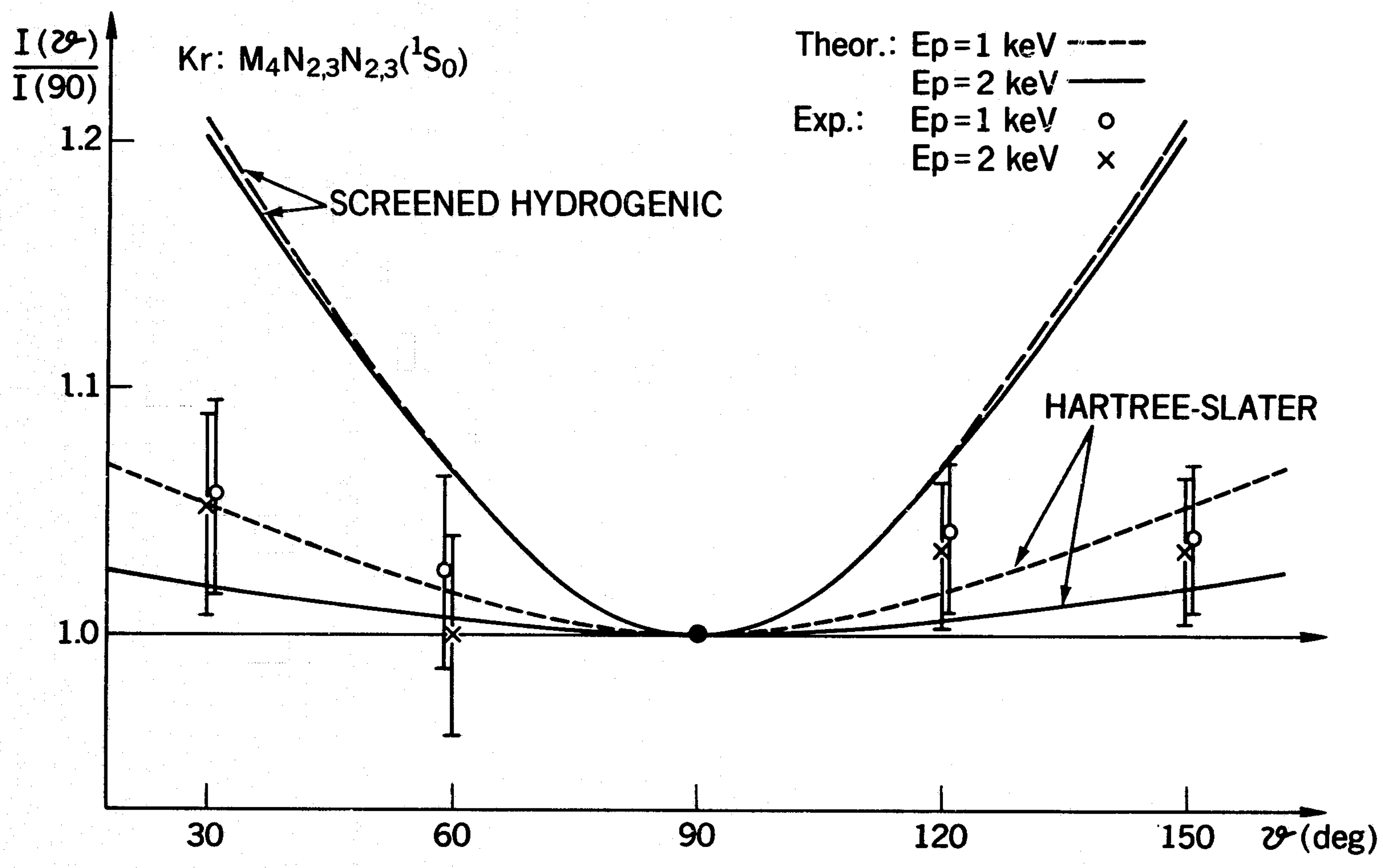
I(ϑ)/I(90)
Kr: $M_4N_{2,3}N_{2,3}(^1S_0)$
Theor.: Ep = 1 keV
Ep = 2 keV
Exp.: Ep = 1 keV
Ep = 2 keV
SCREENED HYDROGENIC
HARTREE-SLATER
1.2
1.1
1.0
30
60
90
120
150
ϑ (deg)

FIGURE 2.

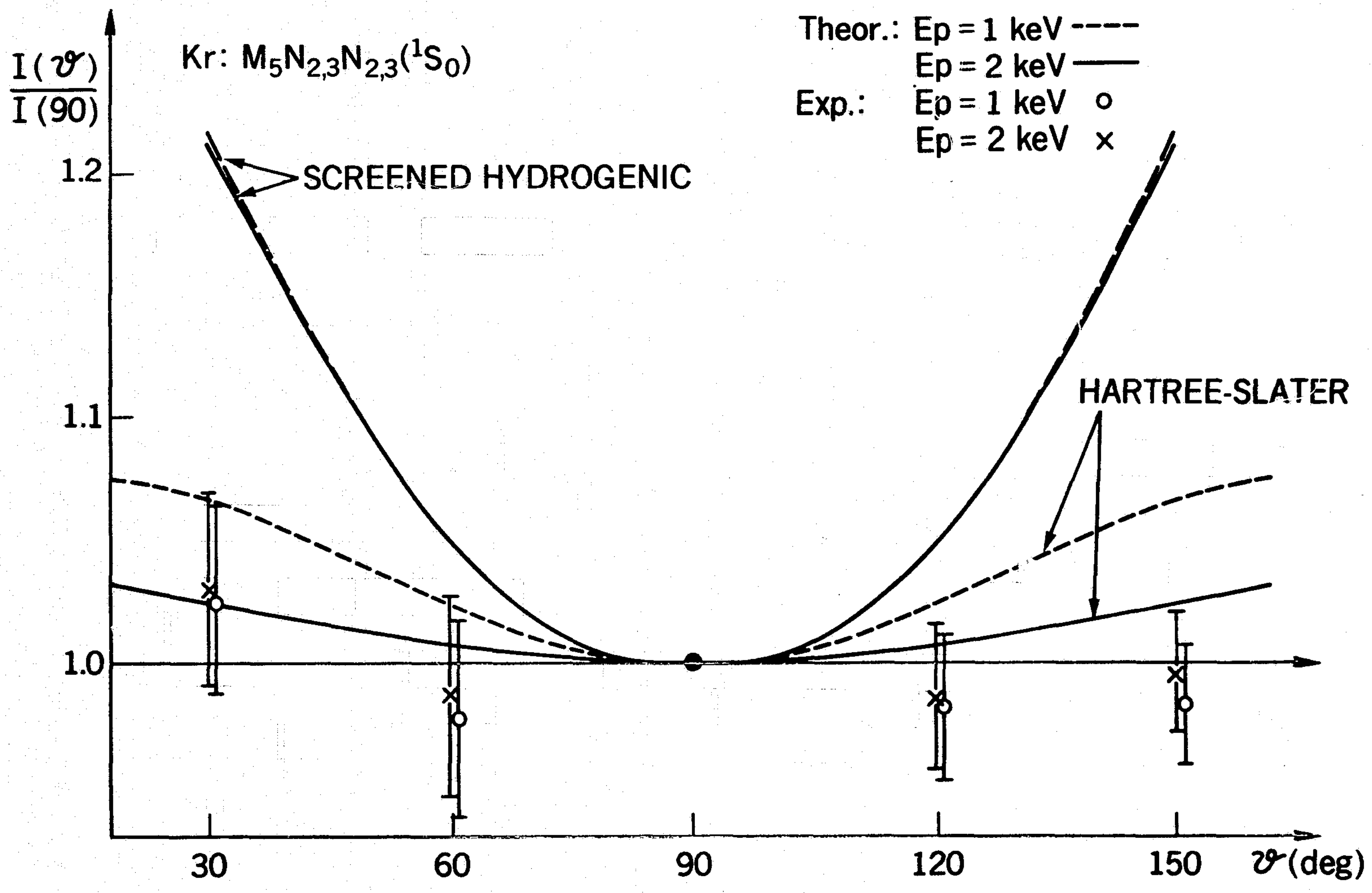
$\frac{I(\vartheta)}{I(90)}$
Kr: $M_5N_{2,3}N_{2,3}(^1S_0)$
Theor.: Ep = 1 keV
Ep = 2 keV
Exp.: Ep = 1 keV
Ep = 2 keV
SCREENED HYDROGENIC
HARTREE-SLATER
1.2
1.1
1.0
30
60
90
120
150
ϑ(deg)

FIGURE 3

Table 1. Values of the ionization cross sections as a function of the impact energies, using Hartree-Slater approximation for the target atom. E(I) and E(eV) are the impact energies in threshold units and eV. $\sigma(m_o)$ is the cross section in units of πa_o^2 for 2 $(2-\delta(m_o,o))$ electrons with the magnetic quantum number m_o. σ_T is the total cross section for the 10 3d shell electrons.

E(I)	E(eV)	$\sigma(m_o=0)$	$\sigma(m_o=\pm 1)$	$\sigma(m_o=\pm 2)$	σ_T
1.2	115	2.53-3†	3.97-3	3.45-3	9.95-3
1.4	134	4.38-3	7.38-3	6.23-3	1.80-2
1.6	155	5.80-3	1.02-2	8.56-3	2.46-2
1.8	173	6.89-3	1.26-2	1.03-2	2.98-2
2.0	193	8.26-3	1.52-2	1.26-2	3.61-2
3.0	290	1.35-2	2.60-2	2.13-2	6.09-2
4.0	386	1.68-2	3.29-2	2.71-2	7.67-2
5.0	483	1.85-2	3.65-2	3.04-2	8.53-2
6.0	580	1.92-2	3.79-2	3.20-2	8.90-2
8.0	773	1.91-2	3.78-2	3.27-2	8.96-2
9.0	869	1.85-2	3.67-2	3.21-2	8.74-2
10.0	966	1.77-2	3.50-2	3.10-2	8.37-2
12.0	1159	1.69-2	3.36-2	3.03-2	8.08-2
15.0	1441	1.54-2	3.06-2	2.82-2	7.42-2
20.0	1921	1.31-2	2.62-2	2.48-2	6.41-2
30.0	2898	1.01-2	2.02-2	2.00-2	5.03-2
3.108	300	1.40-2	2.70-2	2.21-2	6.31-2
5.180	500	1.87-2	3.69-2	3.08-2	8.63-2
10.36	1000	1.79-2	3.56-2	3.16-2	8.51-2
20.72	2000	1.28-2	2.56-2	2.44-2	6.28-2
31.08	3000	9.82-3	1.97-2	1.95-2	4.89-2
36.26	3500	8.74-3	1.75-2	1.76-2	4.39-2

† The fourth digit indicates the power of 10 by which the entry should be raised.