

Calculation of the Inelastic Scattering Factor for the $3p$ to $4s$ Transition in Argon at 40 kv

RUSSELL A. BONHAM^{†*}

*Chemistry Department, Indiana University, Bloomington, Indiana
 and U.S. Naval Research Laboratory
 Washington 25, D.C., U.S.A.*

The results of a calculation of the inelastic electron scattering factor for the excitation of low lying bound states in atoms are presented. Calculations of the detailed shape of the angular intensity for scattered electrons exciting the ($3p^5, 4s^1$) state of Argon have been made and the details are presented. The calculation predicts that the scattering intensity is sensitive to the detailed structure of the radial atomic wave functions in both the ground and excited states.

1. Introduction

With the development of high resolution electron spectrometers it has become possible to measure the inelastic differential scattering cross sections for the electron excitation of the low lying bound states of atoms^{(1), (2), (3)}. At accelerating potentials in the 40 kv region the electron wave length is sufficiently short to allow resolution of the details of the electronic structure. The dependence of the form factors for inelastic scattering from bound states of atoms is then of some theoretical interest since it may be possible to obtain information about the electron distribution in the ground and excited states of atoms and molecules from inelastic scattering experiments. Argon was picked for the purposes of this investigation since Hartree-Fock SCF calculations are available for the wave functions for the ground state and the first excited state ($3p^5 4s^1$)^{(4), (5)}.

2. Theory

If exchange terms are neglected the Schrödinger equation for the inelastic scattering of electrons which excite the p^{th} state of the atom can be written to first order as⁽⁶⁾

$$(\nabla^2 + k_p^2)F^p(\mathbf{r}_0) = \left(\frac{a_0}{a_p}\right)F^0(\mathbf{r}_0)U_{p0}(\mathbf{r}_0) \quad (1.0)$$

where $F^p(\mathbf{r}_0)$ is the scattered amplitude for the p^{th} state, $F^0(\mathbf{r}_0)$ is the scattered amplitude for elastic scattering, a_0 and a_p are Fourier

expansion coefficients for which available experimental evidence indicates that $a_0 \gg a_p (p \neq 0)$ ⁽⁷⁾ and $U_{p0}(\mathbf{r}_0)$ is given as

$$U_{p0}(\mathbf{r}_0) = -\frac{2Z}{a} \left\langle \varphi_N^p(\mathbf{r}) \left| \frac{1}{r-r_0} \right| \varphi_N^0(\mathbf{r}) \right\rangle \quad (1.1)$$

In equation (1.1) " a " is the relativistic Bohr radius, $\varphi_N^p(\mathbf{r})$ is the one electron wave function for the electron involved in the excitation process in the p^{th} state (in this case the $4s$ wave function for argon) and $\varphi_N^0(\mathbf{r})$ is the one electron wave function for the ground state (the $3p$ wave function for argon).

The simplified form for equation (1.1) arises because the ground and excited state wave functions are orthogonal and also because the $3p, 3s, 2p, 2s$ and $1s$ radial wave functions in the ground state are very similar to those in the excited state^{(4), (5)} and for this reason have been assumed to be the same. Effects due to spin have also been neglected. The first Born approximation results in the expression

$$F^p(\mathbf{r}_0) = \frac{\exp(ik_0 r)}{r S_p^2} \left(\frac{2Z a_0}{a a_p} \right) \times \langle \varphi_N^p(\mathbf{r}) | \exp(i\mathbf{S}_p \cdot \mathbf{r}_0) | \varphi_N^0(\mathbf{r}) \rangle \quad (1.2)$$

for the scattered amplitude where S_p is the diffraction variable

$$S_p = \sqrt{k_0^2 + k_p^2 - 2k_0 k_p \cos \theta} \quad (1.3)$$

which for small energy losses is nearly the usual electron diffraction scattering variable S .

For argon equation (1.2) further simplifies to

$$F^p(\mathbf{r}_0) = i\sqrt{3} \frac{\exp(ik_0 r)}{r S_p^2} \left(\frac{2Z a_0}{a a_p} \right) \times \langle \varphi_N^p(\mathbf{r}) | j_1(S_p r) | \varphi_N^0(\mathbf{r}) \rangle \quad (1.4)$$

[†] National Academy of Science—National Research Council—U. S. Naval Research Laboratory Research Associate for the year 1960.

* Contribution No. 1000 from the Chemical Laboratories of Indiana University.

where $j_1(S_{pr})$ is a spherical Bessel function of order 1.

3. Results and conclusions

Equation (1.4) has been evaluated numerically using both Hartree-Fock SCF wave functions^{4),5)} and Slater hydrogenlike one electron functions⁸⁾. The results are shown in Fig. 1. In Fig. 2, the angular dependence of the scattered intensity has been plotted using the Hartree-Fock functions. It is apparent that the use of very approximate wave functions washes out a great deal of the detail in the angular dependence and thus would not be a suitable approximation for inelastic structure investigations. It is also apparent that the inelastic scattering intensity computed from the above approximations contains features dependent on the detailed shape of the ground and excited state wave functions which are in an experimentally accessible region of the scattering curve. Of even greater interest are the facts that, using the above approximations, the inelastic scattering is mainly electron-electron in nature and depends mainly on the excited electron for the case of the excitation of low

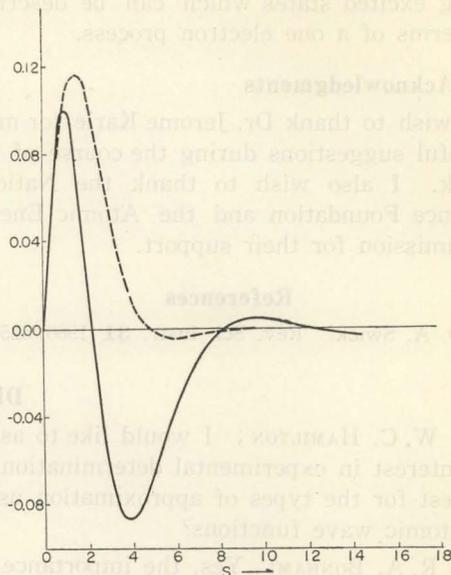


Fig. 1. The Matrix Element

$$\langle \varphi_{4s^1}(r) | j_1(S_{pr}) | \varphi_3^0(r) \rangle$$

for the Excitation of the $3p^5 4s^1$ State of Argon

— Scattering factor calculated using Hartree-Fock SCF radial wave functions.

---- Scattering factor calculated using Slater hydrogen-like radial wave functions.

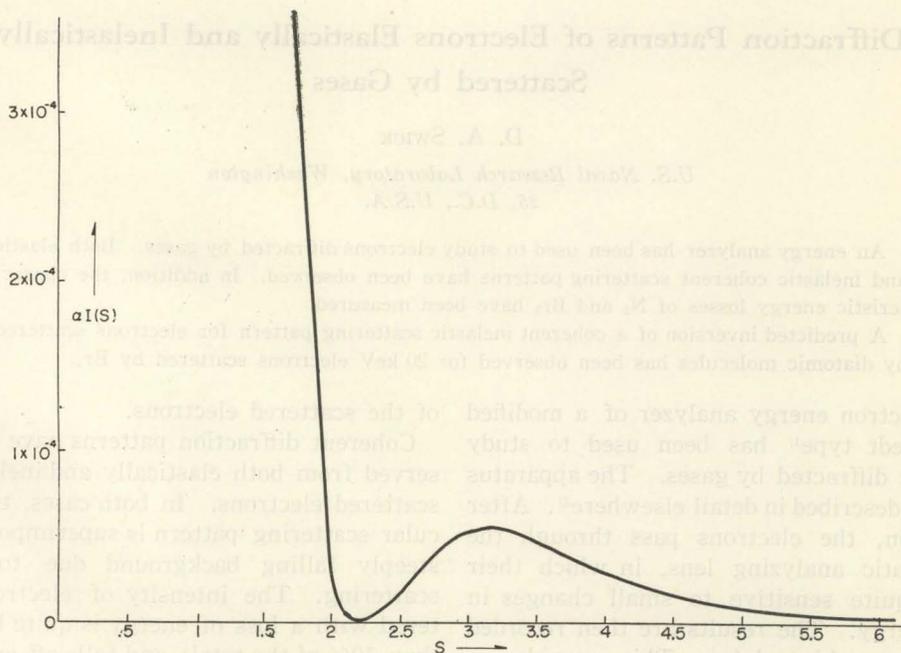


Fig. 2. Plot of the Calculated Angular Intensity for Scattered Electrons Exciting the $(3p^5 4s^1)$ State of Argon.

lying excited states which can be described in terms of a one electron process.

4. Acknowledgments

I wish to thank Dr. Jerome Karle for many helpful suggestions during the course of this work. I also wish to thank the National Science Foundation and the Atomic Energy Commission for their support.

References

1 D. A. Swick: *Rev. Sci. Instr.* **31** (1960) 525.

- 2 G. Möllenstedt: *Z. Naturforsch.* **7A** (1952) 465.
 3 G. Haberstroh: *Z. Phys.* **145** (1956) 20.
 4 D. R. Hartree and W. Hartree: *Proc. Roy. Soc. (London)* **A166** (1938) 450.
 5 R. S. Knox: *Phys. Rev.* **110** (1958) 375.
 6 N. F. Mott and H. S. W. Massey: *The Theory of Atomic Collisions*, (Oxford University Press, London, 1949), 27.
 7 L. S. Bartell and L. O. Brockway: *Phys. Rev.* **90** (1953) 833.
 8 J. C. Slater: *Phys. Rev.* **36** (1930) 57.

DISCUSSION

W. C. HAMILTON: I would like to ask Dr. Bonham whether he thinks that the chief interest in experimental determination of inelastic scattering factors is to provide a test for the types of approximation used in theoretical calculations of excited state atomic wave functions?

R. A. BONHAM: Yes, the importance of conducting such experiments would be to determine experimentally the excited state wave function in cases where the ground state function is known from theory.

JOURNAL OF THE PHYSICAL SOCIETY OF JAPAN
 PROCEEDINGS OF INTERNATIONAL CONFERENCE ON MAGNETISM AND CRYSTALLOGRAPHY, 1961, VOL. II

VOL. 17, SUPPLEMENT B-II, 1962

Diffraction Patterns of Electrons Elastically and Inelastically Scattered by Gases

D. A. SWICK

*U.S. Naval Research Laboratory, Washington
 25, D.C., U.S.A.*

An energy analyzer has been used to study electrons diffracted by gases. Both elastic and inelastic coherent scattering patterns have been observed. In addition, the characteristic energy losses of N_2 and Br_2 have been measured.

A predicted inversion of a coherent inelastic scattering pattern for electrons scattered by diatomic molecules has been observed for 20 keV electrons scattered by Br_2 .

An electron energy analyzer of a modified Möllenstedt type¹⁾ has been used to study electrons diffracted by gases. The apparatus has been described in detail elsewhere²⁾. After diffraction, the electrons pass through the electrostatic analyzing lens, in which their path is quite sensitive to small changes in their energy. The results are then recorded on photographic plates. This provides a measurement of both the magnitude of the energy lost, and of the angular distribution

of the scattered electrons.

Coherent diffraction patterns have been observed from both elastically and inelastically scattered electrons. In both cases, the molecular scattering pattern is superimposed on a steeply falling background due to atomic scattering. The intensity of electrons scattered with a loss of energy is quite low (less than 10% of the total), and falls off extremely rapidly with increasing angle of scattering.

The characteristic energy losses of 20 keV