NOTICE

This report was prepared as an account of work sponsored by the United States Government. Neither the United States nor the United States Department of Energy, nor any of their employees, nor any of their contractors, subcontractors, or their employees, makes any warranty, express or implied, or assumes any legal liability or responsibility for the accuracy, completeness or usefulness of any information, apparatus, product or process disclosed, or represents that its use would not infringe privately owned rights.

ATOMIC EXPANSION METHOD FOR ELECTRON CAPTURE IN ION-ATOM COLLISIONS

C. D. Lin

Kansas State University, Manhattan, Kansas 66506

1

000-2753-104
CONF-781113--36

Introduction

In this presentation I would like to discuss the theory of electron capture in multielectron ion-atom collisions based upon the atomic expansion method proposed by Bates¹ in 1958. For the first time the electron transfer cross sections in ion-atom collisions in the energy range from a few keV/amu to a few MeV/amu collisions can be obtained with good accuracy from ab initio calculations. The presentation will deal primarily with single electron transfer processes; an independent electron approximation including only the electron that is directly transferred will be used. After a brief discussion on the atomic expansion method and its region of validity, the application of the method to the charge transfer in a variety of ion-atom collisions will be discussed. Topics to be included in the talk are: (1) examination of the various first order perturbation theories for charge transfer; (2) the K-K electron capture cross sections in heavy ion-atom collisions; (3) the differential cross sections for electron transfer; (4) electron capture from L- and M-subshells; (5) quasi-molecular binding correction to the atomic expansion method; and (6) further improvement of the theoretical model.

Theory of Electron Capture - the Atomic Expansion Method

The atomic expansion method was first introduced by Bates¹ under the title "Electron Capture in Fast Collisions." However, as we will see later, this theory is practical and useful only for collisions at energies where the projectile velocity is nearly equal to the orbital velocity of the electron to be captured. Nevertheless, the theory does cover a wide range of collision energies since the total electron capture cross section is the sum of contributions from individual subshells of the target atom and the contribution of each subshell peaks near the velocity matching region where the present model works.

In the atomic expansion method, the transfer of a single active electron e from the target A to the projectile B in an encounter

is treated mathematically by solving the time-dependent Schrödinger equation

$$(H_e - i \frac{\partial}{\partial t}) \psi(\vec{r}, t) = 0 \quad (2)$$

by expanding the electronic wave function $\psi(\vec{r}, t)$ in terms of traveling atomic eigenfunctions of $(A+e)$ and of $(B+e)$ systems,

$$\begin{aligned} \psi(\vec{r}, t) = & \sum_m a_m(t) \phi_m(\vec{r}_A) \exp[-i(\frac{1}{2} \vec{v} \cdot \vec{r} + \frac{1}{8} v^2 t + \epsilon_m^A t)] \\ & + \sum_n b_n(t) \phi_n(\vec{r}_B) \exp[-i(-\frac{1}{2} \vec{v} \cdot \vec{r} + \frac{1}{8} v^2 t + \epsilon_n^B t)] \end{aligned} \quad (3)$$

Atomic units are used in (2) and (3) and throughout this article. In (3), ϕ_m and ϕ_n are stationary eigenstates of $(A+e)$ and of $(B+e)$ satisfying

$$[-\frac{1}{2} \nabla_1^2 + V_A(r_1) - \epsilon_m^A] \phi_m(\vec{r}_1) = 0 \quad (4a)$$

and

$$[-\frac{1}{2} \nabla_2^2 + V_B(r_2) - \epsilon_n^B] \phi_n(\vec{r}_2) = 0 \quad (4b)$$

the velocity dependent phase factors are introduced to preserve the translational invariance of (2).

By substituting (3) into (2), using the Hamiltonian

$$H_e = -\frac{1}{2} \nabla^2 + V^A(r_A) + V^B(r_B) \quad (5)$$

where $V^A(V^B)$ is the potential energy of the electron in the field of the target (projectile), a set of first order coupled equations for $\{a_m(t), b_n(t)\}$ are obtained. In an actual calculation, the expansion in (3) is truncated to finite terms. For electron capture problems, the simplest expansion, following (3), with obvious notations, is

$$\begin{aligned} \psi(\vec{r}, t) = & a(t) \phi_A \exp[-i(\frac{1}{2} \vec{v} \cdot \vec{r} + \frac{1}{8} v^2 t + \epsilon_A t)] \\ & + b(t) \phi_B \exp[-i(-\frac{1}{2} \vec{v} \cdot \vec{r} + \frac{1}{8} v^2 t + \epsilon_B t)] \end{aligned} \quad (6)$$

i.e., by including only the initial state ϕ_A of $(e+A)$ and the final state ϕ_B of $(e+B)$

In terms of the simple expansion (6), the coupled equations for $a(t)$ and $b(t)$ are

$$\begin{aligned} i(1-s^2)\dot{a} = & a(h_{AA}-s_{AB}h_{BA}) + b(h_{AB}-s_{AB}h_{BB})e^{i\omega t} \\ i(1-s^2)\dot{b} = & b(h_{BB}-s_{BA}h_{AB}) + a(h_{BA}-s_{BA}h_{AA})e^{-i\omega t} \end{aligned} \quad (7)$$

where s_{ij} is the overlap matrix element between the nonorthogonal basis functions ϕ_A and ϕ_B , h_{ij} ($i, j = A, B$) is the matrix element of V^A or of V^B , $s^2 = s_{AB}s_{BA}$ and $\omega = \epsilon_A - \epsilon_B$. The explicit definitions of these matrix elements are given in Eqn. (6) of Ref. 2.

It is to be emphasized that the expansion in (6) is a truncated basis expansion; it is applicable to problems where the capture probability is not small.

Region of Validity

The two-state, two-center atomic expansion (6) and (7) have been applied to $p + H(1s) \rightarrow H(1s) + p$ and to $p + He(1s^2) \rightarrow H(1s) + He^+(1s)$ collisions with results which agree with experimental data and with more sophisticated calculations over a certain energy region.³ The method is known to be not valid for collisions at very high energies, nor for the capture to the excited states. From the calculations performed by different workers, it is known that adding more basis functions of excited states in the atomic expansion does not improve the convergence significantly.⁴ To obtain greater accuracy, it was concluded that continuum states have to be included. This is achieved in the $p + H \rightarrow H + p$ collisions by including pseudo-states⁵ or by using Sturmian basis functions⁶ in the atomic expansion, but these methods are

MASTER

DISCLAIMER

This report was prepared as an account of work sponsored by an agency of the United States Government. Neither the United States Government nor any agency Thereof, nor any of their employees, makes any warranty, express or implied, or assumes any legal liability or responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights. Reference herein to any specific commercial product, process, or service by trade name, trademark, manufacturer, or otherwise does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States Government or any agency thereof. The views and opinions of authors expressed herein do not necessarily state or reflect those of the United States Government or any agency thereof.

DISCLAIMER

Portions of this document may be illegible in electronic image products. Images are produced from the best available original document.

difficult to generalize to other systems.

The region of validity of the atomic expansion method is rarely discussed. In the limit of $v = 0$, expansion (6) is an expression for the linear combination of atomic orbitals (LCAO) for the evaluation of the two molecular potential curves which converge to ϵ_A and ϵ_B at large R , the internuclear separation. To see this, we notice that by making a proper phase transformation, the diagonal terms on the right hand side of (7) can be eliminated, resulting

$$\begin{aligned} i \dot{d}_A &= d_B e^{i(\omega t + \delta)} (h_{AB} - s_{AB} h_{BB}) / (1 - s^2) \\ i \dot{d}_B &= d_A e^{-i(\omega t + \delta)} (h_{BA} - s_{BA} h_{AA}) / (1 - s^2), \end{aligned} \quad (8)$$

where d_A (d_B) is related to $a(b)$ by a phase transformation. In (8), $\omega t + \delta$ is given by

$$\begin{aligned} \omega t + \delta &= \int_{-\infty}^t \{ [\epsilon_A + (h_{AA} - s_{AB} h_{BA}) / (1 - s^2)] \\ &\quad - [\epsilon_B + (h_{BB} - s_{BA} h_{AB}) / (1 - s^2)] \} dt, \end{aligned} \quad (9)$$

which is the time integral of the two "potential curves" obtained in the atomic expansion method.⁷

In Fig. 1, we show the two lowest potential

curves for the $F^{9+} - Si$ system, obtained by assuming that the Hamiltonian is

$$H_e = -\frac{1}{2} \nabla^2 - \frac{Z_A}{r_A} - \frac{Z_B}{r_B} \quad (10)$$

The solid lines correspond to the "adiabatic" molecular curves while the dashed lines correspond to the two terms in the square brackets of (9) [notice that the matrix elements in (9) are velocity dependent and are complex numbers, but at low velocities the differences at different v are negligible and the imaginary components are very small]. We note that the differences of the two sets of curves at large R are not significant, thus the atomic expansion method provides an adequate description for the distortion of the active electron in the field of the projectile and the target at large R . On the other hand, the two sets of curves at small R differ significantly. For collisions at small impact parameters, the small R region is important but the potential curves in the atomic expansion method do not converge to the

the adiabatic molecular limit as $v \rightarrow 0$; thus the atomic expansion method is not expected to be valid for small v .

The translational factor which describes that the electron is moving with the projectile or with the target is properly accounted for in the atomic expansion (3), thus the atomic expansion method is expected to be valid for region of R where the distortion of the active electron is properly treated, i.e., in the large R region. For projectiles with velocity near the orbital K-shell electron velocity, the capture occurs primarily near the K-shell radius and the present method is expected to work -- as demonstrated from the results to be presented in the next few sections. For slower collisions, the exponents of the oscillating term $\exp \pm i(\omega t + \delta)$ in (7) are large and the calculation is very sensitive to the proper treatment of the distortion of the electron due to the two nuclei. For faster collisions the capture has to occur at small R where the distortion of the electron by the two nuclei is again not properly treated by the expansion (6) and thus the atomic expansion method is not valid at high velocities.

Despite the above limitations, the atomic expansion method is still very useful in describing the charge transfer processes in a variety of situations of practical interest. In the following I will describe several of these applications.

A Perturbation Theory for Charge Transfer?

According to the very publicized unpublished results of Drisco,⁸ the second Born term is more important than the first Born term in the perturbation expansion for charge transfer in the high-energy limit. The question is then: is there a first order perturbation theory for charge transfer?

Because of the nonorthogonality of initial and final states in the electron capture process, there are at least two well-known versions of first Born theories: the Oppenheimer, Brinkman and Kramers⁹ (OBK) approximation, and the Jackson and Schiff¹⁰ (JS) approximation. The validity of these two approximations has been a topic of constant discussion over the years. To understand the origin of the confusion,² we note that in (8) if the capture amplitude is small, we can set $d_A \approx 1$ in the second equation. By neglecting δ and assuming $s^2 \ll 1$, the capture amplitude can be written as

$$\begin{aligned} d_B(+\infty) &\sim \int_{-\infty}^{\infty} dt \int d^3r \phi_B \left[-\frac{Z_B}{r_B} - h_{AA} \right] \phi_A \\ &\quad \times \exp(-i(\vec{v} \cdot \vec{r} + \omega t)) \end{aligned} \quad (11)$$

where

$$h_{AA} = \frac{Z_B}{R} [-1 + (1 + Z_A R) e^{-2Z_A R}] \quad (12)$$

for the K-K capture. The extra term included in h_{AA} is due to the nonorthogonality of initial and final states. If h_{AA} is arbitrarily set to zero, we obtain the OBK approximation. On the other hand, in the case of $Z_A = Z_B = 1$, if we choose $-h_{AA} = 1/R$ -- its large R limit value, then the term included in $-h_{AA}$ resembles the internuclear interaction considered in the JS approach. From our derivation, however, this term is not an internuclear interaction term. In particular, with $Z_A \neq 1$, the large R limit of $-h_{AA}$ is not $Z_A Z_B / R$, the internuclear potential, but is Z_B / R . The unphysical prediction of JS approximation¹¹ for $Z_A \neq 1$ can thus be explained.

When the capture probability is small, the capture cross section computed from (11) is equal to that calculated from the two-state atomic expansion method. Equation (11) can also be obtained from the first order perturbation theory by requiring the final state wave function to be orthogonal to the initial state wave function; it is equivalent to the distorted wave theory of Bassel and Gerjuoy.¹² In this connection, however, eq. (11) is valid only in the region where the two-state atomic expansion method is also valid (in addition to the requirement of small capture probability). In particular, it reduces to the OBK approximation at high energies. However, in the energy region where the cross section peaks, the "first order" expression (11) appears adequate.

In Fig. 2 we compare the theoretical and experimental electron capture cross sections from the K-shell

of Ar atoms by protons to assess the validity of theoretical models. The experimental data, shown in open circles, are from Macdonald *et al.*¹³ The OBK results are a factor of three too high. The modified first Born theory, called Born(C) method by its original authors,¹⁴ predicts cross sections in good agreement with experimental data at the high energy side, but not on the low energy side. Similarly, the continuous-distorted-wave results of Belkić and McCarroll¹⁵ fails at low energies, though the agreement at high energies is good. The results of the two-state, two-center atomic expansion method, shown in the solid line, agree reasonably well with experimental data, both in magnitude and in shape. The origin of the remaining discrepancy will be further discussed later.

K-K Capture for Heavy Ion-Atom Collisions

It was emphasized earlier that the two-state atomic expansion method is not a perturbation approximation; it is useful for evaluating electron capture cross sections for near-symmetric collisions where the cross sections are large. In Table I we present the results of some of these calculations and the comparison with experimental data; the general agreement between the present theory and experiment is noted.

Table I

K-K electron capture per target electron (in 10^{-20} cm^2). For source of experimental data, see Ref. 16.

Projectile + Target	Energy (MeV)	V/V_K^{**}	σ_{CAL}	$\sigma_{\text{EXP}}^{\dagger}$
$\text{N}^{7+} + \text{Ne}$	14	.79	368	355
	19	.92	343	350
$\text{O}^{8+} + \text{Ne}$	24	.96	368	435
	30	1.08	269	330
	35	1.17	195	300
$\text{F}^{9+} + \text{Ne}$	20	.81	516	440
	25	.90	440	430
	30	1.00	360	410
$\text{C}^{6+} + \text{Ar}$	12.6	.42	1.30	1.79
	19.0	.52	2.52	2.34
	22.6	.57	5.40	5.83
$\text{N}^{7+} + \text{Ar}$	14.7	.42	5.1	3.2
	26.3	.56	12.6	13.2
$\text{F}^{9+} + \text{Ar}$	20	.42	25.2	9.7
	30	.52	32.4	29.0
	36	.57	45.6	30.4
	46	.64	52.8	47.7
	56	.71	48.8	53.6
	66	.77	40.8	48.8
	76	.82	39.6	44.3
$\text{F}^{9+} + \text{Kr}$	46	.30	7.4(-2)	1.0(-2)
	56	.33	7.9(-2)	3.7(-2)
	66	.36	7.5(-2)	6.4(-2)
	76	.39	6.8(-2)	6.1(-2)
$\text{Cl}^{17+} + \text{Kr}$	100	.33	1.55	.60
	120	.36	1.40	1.15
	140	.39	1.62	1.90
	160	.42	2.50	2.8

^{**} Projectile velocity with respect to the orbital velocity of the K-shell electron defined by $V_K = \sqrt{2I_K}$, where I_K is the K-shell ionization energy of the target.

[†] Typical experimental uncertainty is of the order of 20%.

Differential Cross Sections for Charge Transfer

Differential cross sections for electron capture in ion-atom collisions often exhibit detailed information not evident in the integrated cross sections. According to the first Born theories proposed by Omidvar *et al.*¹⁴ and by Halpern,¹⁷ there is a dip structure in the differential cross sections for electron capture. To confirm this prediction, Cocke *et al.*¹⁸ measured the differential cross sections for the electron transfer in p-Ar collisions at 6 MeV and Bratton *et al.*¹⁹ measured the differential cross sections in p-He collisions at 293 keV. In both experiments, the differential cross sections show monotonic decrease with increasing scattering angles without any evidence of structure as predicted by the theory.¹⁷

The drawbacks of the various first Born theories for charge transfer have been discussed earlier.² To show that the atomic expansion method is adequate in describing the differential cross sections, we show in Fig. 3 the differential cross sections for electron capture from the K shell of Ar atoms by 6 MeV protons. The experimental data are from Cocke *et al.*¹⁸ the Born(C) curve is due to the prediction of Omidvar *et al.*¹⁴ the dashed lines are due to Belkić and Salin,²⁰ using OBK approximation for the charge transfer amplitude and the results of the two-state, two-

center atomic expansion method are shown in a solid line.²¹ It is clear that the atomic expansion method does predict differential cross sections very well also.

The atomic expansion method is usually formulated in the impact parameter approximation and, in actual calculations, a straight line trajectory is usually assumed for fast collisions. To obtain differential cross sections, an eikonal approximation for the motion of the heavy particle is employed. The resulting equation for the differential cross sections is

$$\frac{d\sigma}{d\Omega} = \left| i\mu v \int_0^\infty \rho^{1+2i\nu} J_0(2\mu v p \sin \frac{\theta}{2}) b(\rho) d\rho \right|^2 \times (a_0^2 s_r^{-1}) \quad (13)$$

where μ is the reduced mass of the projectile, v is the velocity. J_0 is the zeroth Bessel function, ν is the eikonal phase obtained from treating the nuclear motion semiclassically and $b(\rho)$ is the capture amplitude calculated from the impact-parameter approximation. In Fig. 3, the calculations of Belkic and Salin²⁰ and of Lin and Soong²¹ both use the eikonal phase assuming Coulomb interaction between the proton and Ar nucleus interaction; on the other hand, the former uses OBK amplitude for $b(\rho)$ and the latter uses $b(\rho)$ calculated from the atomic expansion method.

Electron Capture from L- and M-Subshells

At smaller projectile energies, electron capture cross sections are dominated by the capture from the outer subshells. To study electron transfer from subshells other than the K shell within the independent electron approximation, a realistic atomic potential has to be employed.

The atomic potential we choose for this purpose

is the Herman-Skillman potential.²² For simplicity we consider the capture of electrons from various subshells of Ar atoms by protons. In this case, the atomic potentials used in (5) are $V_B = -1/r_B$ and $V_A = V_{HS}(r_A)$ where V_{HS} is fitted to the numerical Herman-Skillman potential assuming an analytic form

$$V_{HS}(r) = -\frac{1}{r} [1 + (Z-1)e^{-\lambda r} \times (1 + a_1 r + a_2 r^2 + a_3 r^3)] \quad (14)$$

where $Z=18$ for Ar. The functional form (14) is chosen so that the matrix element h_{AB} can be conveniently evaluated. The initial wave function ϕ_A is represented in a form

$$\phi_A = \sum_1 C_1 U_1 \quad (15)$$

where U_1 is a Slater basis function chosen similar to that used in the analytic Hartree-Fock wave functions.²³ The expansion coefficients $\{C_1\}$ are obtained by solving (4a). In Fig. 4 the total electron capture cross sections of Ar by protons in the 1 keV - 3 MeV region are shown. The theoretical values for the L-shell contribution are also shown in the 0.2-3.0 MeV region. We notice that the theoretical values are slightly higher than experimental data,²⁴ but the general agreement is good.

It was pointed out in the paragraph following equation (9) that the exponent $\omega t + i\delta$ in the coupled equation (8) is the time integral of the difference of the two "potential curves" obtained in the atomic expansion method. The two "potential curves" do not converge to the adiabatic molecular potential curves in the $v = 0$ limit. For collisions at lower energies, the oscillatory exponential in (8) is the dominating factor for determining the magnitude of the coupling. As v decreases, the quasi-molecular behavior of the collision system can be taken into account simply by replacing $\omega t + i\delta$ by the time integral of the difference of the two relevant adiabatic molecular curves. In Fig. 5, we compare the electron transfer cross sections of F^{9+} - Si collisions.⁷ The experimental data of Tawara et al.²⁵ at low energies are better explained by the quasi-molecular model (dashed line) than the two-state calculation where no binding correction has been included (solid line). At higher energies, the two theoretical models do not have difference. The two sets of potential curves are shown in Fig. 1.

Further Improvement of the Theoretical Model

From the above discussion, it is clear that the simple two-state, two-center atomic expansion method, when combined with a suitable independent electron model, provides an adequate description for single electron transfer processes in the energy region where the model is expected to work. Further improvement involves both the atomic model as well as the scattering model.

A) The scattering model: For asymmetric systems, like the K-K capture in p-Ar collisions, improvement of the theory and experiment at lower energies might be achieved by including a few more atomic states of the target in the expansion. Work is underway to investigate this effect. For more symmetric systems, a

three-center atomic expansion method is a desirable first step toward understanding collisions at small impact parameters. In this method, expansion using the eigenfunctions of the united atom around the third center -- the center of the two charges, is introduced to describe the distortion of the electron at small R which is not adequately described by the truncated two-center expansion. This appears to be a very reasonable theoretical model, but the progress is hampered by numerical complications.

B) The atomic model: Within the independent electron approximation, other model potentials can be used, but no significant change is expected. Additional refinement, within the two-center expansion method, can be achieved by using the total many-electron Hamiltonian and wave functions of the colliding system. At low energies this multielectron model is expected to result in some difference from the independent electron model.

It must be emphasized that great care must be taken in comparing theoretical electron transfer cross sections with experimental data if accurate comparison is desirable. Experimental data are often deduced from x-ray data or Auger electron data alone. There are almost no experiments in which x-ray and Auger electrons are both measured. Since the production of inner-shell vacancy is often accompanied by outer-shell vacancies, only the average fluorescence yield ω is well defined. This average ω has to be measured directly in the experiment when the structure of x-ray or Auger-electron data is not resolved. Since it is impossible to treat multiple vacancy production cross sections adequately in the present theory, it is premature to claim very high accuracy in comparing the theory with experiments.

It is appropriate to comment that in Fig. 2 the K-shell electron of Ar can be transferred to the proton in two different ways: a direct capture process; and a two-step process in which an L-shell electron is captured by the proton, accompanied by a direct excitation of the K-shell electron to the L shell. These two processes cannot be distinguished experimentally. The experimental data of Fig. 2 for the K-K capture are obtained by subtracting the two-step cross sections from the measured total electron transfer cross sections. This method can cause significant errors since the two processes described above should be treated coherently. A more suitable approach is to include both processes in the theoretical model and compare the results with the experimental total electron transfer cross sections.

References

1. D. R. Bates, Proc. R. Soc. A **724**, 294 (1958).
2. C. D. Lin, S. C. Soong and L. N. Tunnell, Phys. Rev. A **17**, 1646 (1978).
3. See the reviews by B. H. Bransden, Rep. Prog. Phys. **35**, 949 (1972); D. Basu, S. C. Mukherjee and D. P. Sural, Phys. Rept. **42C**, 147 (1978).
4. L. Wilets and D. F. Callagher, Phys. Rev. **147**, 13 (1966).
5. I. M. Cheshire, D. F. Callagher and A. J. Taylor, J. Phys. B **3**, 813 (1970).
6. R. Shakeshaft, Phys. Rev. A **14**, 1626 (1976).
7. C. D. Lin, J. Phys. B, to be published.
8. R. M. Drisko, thesis (Carnegie Institute of Technology, 1955) unpublished.
9. J. R. Oppenheimer, Phys. Rev. **31**, 349 (1928); H. C. Brinkman and H. A. Kramers, Proc. Acad. Sci. (Amsterdam) **33**, 973 (1930).
10. J. D. Jackson and H. Schiff, Phys. Rev. **89**, 359 (1953).

11. A. Halpern and J. Law, Phys. Rev. Lett. 31, 4 (1973); Y. B. Band, Phys. Rev. Lett. 37, 634 (1976).
12. R. H. Bassel and E. Gerjuoy, Phys. Rev. 117, 749 (1960).
13. J. R. Macdonald, C. L. Cocke and W. W. Eidson, Phys. Rev. Lett. 32, 648 (1974).
14. K. Omidvar, J. E. Golden, J. H. McGuire and L. Weaver, Phys. Rev. A 13, 500 (1976).
15. Dz Belkić and R. McCarroll, J. Phys. B 10, 1933 (1977); see also footnote 35 of Ref. 2.
16. C. D. Lin, J. Phys. B 11, L185 (1978).
17. H. A. Halpern, Phys. Rev. A 15, 619 (1976).
18. C. L. Cocke, J. R. Macdonald, B. Curnutte, S. L. Varghese, and R. Randall, Phys. Rev. Lett. 36, 782 (1976).
19. T. Bratton, C. L. Cocke and J. R. Macdonald, J. Phys. B 10, L517 (1977).
20. Dz Belkić and A. Salin, J. Phys. B 9, L397 (1976). See footnote 25 of Ref. 22.
21. C. D. Lin and S. C. Soong, Phys. Rev. A 18, 499 (1978).
22. F. Herman and S. Skillman, Atomic Structure Calculations (Prentice-Hall, Englewood Cliffs, N. J., 1963).
23. E. Clementi and C. Roetti, Atomic Data and Nuclear Data Tables 14, 177 (1974).
24. From the compiled data of H. Tawara and A. Russek, Rev. Mod. Phys. 45, 178 (1973).
25. H. Tawara, P. Richard, T. J. Gray, J. Newcomb, K. A. Jamison, C. Schmiedekamp and J. M. Hall, to be published in Phys. Rev.