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Theoretical K-Shell Auger Rates, Transition Energies, and Fluorescence Yields for Multiply Ionized Neon*

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X-ray rates, Auger group rates, and X-shell fluorescence yields are presented for variously ionized states of neon. The nonrelativistic Hartree-Fock-Slater atomic model, with the exchange approximation of Herman-Van Dyke-Ortenburger, is used. The x-ray and Auger transition energies were obtained by the adiabatic method. The theoretical results presented here are applicable to the analysis of defect configurations which may be produced in a heavy-ion-neon collision. It is shown that the commonly used statistical scaling procedure to obtain the K-shell fluorescence yield for defect configuration leads to significant errors for neon.

I. INTRODUCTION

The deexcitation of an atom with an inner-shell vacancy can occur mainly by two independent competing processes: (a) the emission of x rays and (h) the ejection of Auger electrons. The fluorescence yield for a K -shell vacancy is defined as

 $\omega_{\kappa} = \Gamma_{\kappa}/(\Gamma_{\kappa} + \Gamma_{A}),$

where Γ_x and Γ_A are the total x-ray rate and the total Auger rate, respectively. The theoretical values of Γ_x and Γ_A (and therefore, ω_x) depend upon the electronic configuration of the atom.

When the inner-shell vacancy is produced in an atom without changing the electronic configura-

tion in other shells, the theoretica1 results, which have been already reported by McGuire¹ and by tion in other shells, the theoretical results, which
have been already reported by McGuire¹ and by
Bhalla and co-workers,^{2,3} can be used. Calcula tions in Refs. 1-3 are with the nonrelativistic Hartree-Pock-Slater (HFS) model and are for the K shell, L subshells, and M subshells. Such calculations were first performed by Rubenstein. ' Recently, extensive calculations of ω_r and ω_r using screened hydrogenic wave functions, were reported by Kostroun et al .⁵ Earlier theoretical values obtained by using the hydrogenic wave functions with (and without) screening parameters also appear in the literature. $6 - 8$

Relativistic calculations of the Auger rates with the statistical Thomas-Fermi model, 9 with the nonrelativistic HFS potential,¹⁰ and with the

 $\emph{relativistic HFS model^{11–13} have been performance$ for K -shell vacancies. X-ray rates to the K -shell and L -subshell vacancies have been calculated by
Scofield¹⁴ and by Rosner and Bhalla.¹⁵ where the Scofield¹⁴ and by Rosner and Bhalla,¹⁵ where the effects of retardation were included and selfconsistent relativistic HFS wave functions were used. Bhalla¹⁶ extended these calculations for the M subshells.

It should be noted that the calculations referred to above, whether nonrelativistic or relativistic in nature, are not appropriate when an innershell vacancy is produced in a heavy-ion collision: several additional electrons are stripped from the atom (in addition to the creation of an innershell vacancy) in violent heavy-ion collisions. The relevant experimental data are (a) experimental observations of the charge-state distrimental observations of the charge-state distri-
butions,¹⁷ (b) increase in x-ray transition enerbutions,¹⁷ (b) increase in x-ray transition energies¹⁸⁻²⁴ as compared to normal x-ray energies,²⁵ (c) decrease in Auger-electron energies,²⁶ (d) the e**r**
26 (c) decrease in Auger-electron energies,²⁶ (d) the appearance of both satellite¹⁹⁻²⁰ and hypersatellite $K\alpha$ lines, and (e) significant deviations of experimental fluorescence yields^{28,29} from the norma
values.³⁰ values.³⁰

In order to identify the possible electronic configurations which can lead to shifts in the x-ray and Auger energies, the relative intensities of x rays (for example, $K\alpha/K\beta$), and the satellite and hypersatellite structure, explicit calculations with a realistic atomic model are needed. The importance of such calculations is emphasized by another set of experiments, in which the cross section of a particular x-ray production process, $\sigma_{\gamma}(E)$, is measured as a function of the bombarding energy E of the heavy ion. Several groups³¹

FIG. 1. Percentage deviation of the $(2p-1s)$ x-ray rate computed with the statistical scaling procedure from our explicit HFS calculation vs the number of electrons in the $2p$ shell for various electronic configurations of neon.

have reported such measurements of $\sigma_x(E)$ for a range of incident energies and combinations of projectiles and target materials. The theoretical projectiles and target materials. The theoretica
models³²⁻³⁶ predict the cross section for creatin a vacancy, $\sigma_I(E)$. Comparison of the theoretical $\sigma_I(E)$ can be made with $\sigma_x(E)/\omega_I$, where ω_I is the appropriate fluorescence yield, which depends on the relevant electronic configuration before the deexcitation of the vacancy occurs.

Recently, Larkins³⁷ has estimated the effects on ω_{K} and ω_{2b} of argon of various electron configurations. This was done by applying scaling factors to the x-ray and Auger rates calculated for the normal argon configuration with only one for the normal argon configuration with only or
vacancy. Fortner *et al*.³⁸ have reported simila calculations for copper. For several configurations of argon, Bhalla and Walters³⁹ have explicitly calculated the x-ray rates, Auger rates, and fluorescence yields. Significant deviations between the statistical scaling procedure³⁷ and the explicit calculations³⁹ were found for several cases in argon.

In this paper we present theoretical x-ray rates, Auger rates, and K -shell fluorescence yields for multiply ionized neon, and critically examine the approximate statistical scaling procedure for neon.

FIG. 2. Ratio of the square of the $K\alpha$ x-ray matrix element for various defect configurations and the square of the matrix element for the configuration with only one K-shell vacancy vs the number of electrons in the $2p$ shell.

Section II contains a description of the theoretical model used in the calculations, followed by numerical results in Sec. III. Our calculations are compared with the statistical scaling procedure in Sec. IVA, and with the experimental data in Sec. IVB.

II. THEORY

The bound-state one-electron wave functions defined below are used in the calculation of the x-ray rates. These are also used with appropriate continuum-state wave functions in the computation of the Auger rates. Atomic units $(\hbar = m_e = e = 1)$ are used throughout the following development.

A. Bound- and Continuum-State Wave Functions

The one-electron wave functions are solutions of the Schrödinger equation

$$
\left(-\frac{1}{2}\nabla^2 + V(r) - \epsilon\right)\phi(\vec{r}) = 0.
$$
 (1)

The spherically symmetric potential function $V(r)$ is specified for an atom of atomic number Z by the shell occupation numbers $N(n, l)$ in terms of the hydrogenic principal quantum number n and angular momentum quantum number l . Thus, the total number of electrons in the configuration

FIG. 3. Percentage deviation of the total K -shell Auger rates computed with the statistical scaling procedure from our explicit HFS calculations vs the number of electrons in the $2p$ shell for various electronic configurations of neon.

is $Z_0 = \sum_{n,i} N(n, l)$. No attempt is made to consider such details as would arise from the explicit inclusion of many-electron coupling schemes for open shells. The potential used in the present work is defined below.

In terms of the spatial part of the one-electron bound-state functions of form $\phi_{nlm}(\tilde{r}) = P_{nl}(r) Y_{lm}(\hat{r})/$ $r,$ a density ρ is defined as

$$
4\pi r^2 \rho(r) = \sum_{n l} N(n, l) P_{n l}^2(r).
$$

A potential function is then defined as the sum of two terms,

$$
V'(r) = V_d(r) + V_x(r) ,
$$

where the direct term is

$$
V_d(r) = -\frac{Z}{r} + \int \frac{\rho(\vec{\mathbf{r}}')}{|\vec{\mathbf{r}} - \vec{\mathbf{r}}'|} d^3 r',
$$

and the exchange term

 $V_x(r) = -2[3\rho(r)/8\pi]^{1/3}(1+\text{tanh}G)$

includes a dimensionless inhomogeneity correction factor to the Slater-type exchange approximation where

FIG. 4. Percentage deviation of the K-shell fluorescence yield computed with the statistical scaling procedure from our explicit HFS calculations vs the number of electrons in the $2p$ shell for various electronic configurations of neon with a single K -shell vacancy.

$$
G = \frac{\beta [2(\nabla \rho/\rho)^2 - 3\nabla^2 \rho/\rho]}{\rho^{2/3}}.
$$

The parameter $\beta = 0.0028$, consistent with the optimum choice suggested by Herman and optimum choice suggested by Herman and
Schwarz,⁴⁰ is used for all calculations. The fina potential function is obtained by appending to $V'(r)$ as defined above, a "latter tail" correction:

$$
V(r) = \begin{cases} V'(r) , & -V'(r) > (Z - Z_0 + 1)/r \\ - (Z - Z_0 + 1)/r , & -V'(r) < (Z - Z_0 + 1)/r \end{cases}.
$$

The occupied bound-state radial functions P_{nl} are self-consistent solutions of the Schrödinger equation (1) calculated as described by Herman equation (1) calculated as described by Herman
and Skillman.⁴¹ Excited (unoccupied) bound-stat and continuum-state radial functions are calculated with the same potential.

The motivation for including the inhomogeneity corrections in the local-exchange approximation is that it does provide significant corrections in the high-electron-density regions near the nucleus. The over-all gross effect of the inhomogeneity correction is to tend to concentrate charge density nearer the nucleus and in this sense make the oneelectron functions more correlated.

B. Transition Rates

Consider one inner-shell vacancy designated by n_3l_3 in an atom with atomic number Z and with N electrons. The total Hamiltonian H can be written (ignoring the spin-orbit coupling term) as

$$
H=H_0+H'
$$

with

$$
H_0 = \sum_{i=1}^{N} \left[-\frac{1}{2} \nabla_i^2 - Z / r_i + V(r_i) \right],
$$

$$
H' = \sum_{i \ge 1} 1 / r_{ij} - \sum_{i} V(r_i).
$$

The central-field potential $V(r_i)$ is the sum of the average electron-electron interaction and the exchange potential in the Herman-Van Dyke-Ortenburger approximation, as discussed in Sec. IIA.

We denote by ϕ_i , the initial state with a vacancy n_3l_3 . The final state ϕ_f after the Auger transition contains two new vacancies and an electron in the continuum. Consider ϕ_i and ϕ_f as properly antisymmetrized wave functions. The standard perturbation theory gives for the total Auger transition rate

$$
\Gamma_A = 2\pi \overline{\sum} \left| \langle \phi_f(1,2,\ldots,N) \, | \sum_{i \geq j} \frac{1}{r_{ij}} \, | \, \phi_i(1,2,\ldots,N) \rangle \right|^2.
$$

The density of final states is unity when the continuum-state wave function is normalized in

the energy scale, as is done in the present work. The symbol $\overline{\Sigma}$ denotes the average and the sum over the initial and the final states, respectively.

It is more convenient to rewrite the total Auger rate Γ_A as a sum of the various possible Auger group rates. The Auger group rate for the transition involving two electrons, initially described by $n_1 l_1$ and $n_2 l_2$, filling the vacancy $(n_3 l_3)$ and resulting in one electron in the continuum $EI₄$ is

$$
T_A(n_3l_3 + n_1l_1, n_2l_2) = 2\pi N_{12} \sum | \mathfrak{M} |^2 , \qquad (2a)
$$

$$
\mathfrak{M} \equiv \langle \phi(n_3 l_3, E l_4) | 1/r_{12} | \phi(n_1 l_1, n_2 l_2) \rangle. \tag{2b}
$$

The two-electron antisymmetrized wave function ϕ in the above equation can be described by the LSJM coupling scheme or other coupling scheme. The Auger group rates are independent of the choice of the coupling schemes. The weighting factor N_{12} in Eqs. (2) is given in terms of the $n_2 l_2$ orbitals⁴² by

occupation numbers
$$
N_1
$$
 and N_2 for the $n_1 l_1$ and
\n $n_2 l_2$ orbitals⁴² by
\n
$$
N_{12} = \frac{N_1 N_2}{(4l_1 + 2)(4l_2 + 2)}
$$
 for inequivalent electrons,
\n
$$
= \frac{N_1 (N_1 - 1)}{(4l_1 + 2)(4l_1 + 2 - 1)}
$$
 for equivalent electrons
\n
$$
(N_1 = N_2, n_1 = n_2, l_1 = l_2).
$$
 (3)

FIG. 5. Percentage deviation of the K -shell fluorescence yield computed with the statistical scaling procedure from our explicit HFS calculations vs the number of electrons in the $2p$ shell for various electronic configurations of neon with a double K -shell vacancy.

 $\overline{8}$

$$
\mathfrak{M} \equiv \langle \phi(n_3l_3, El_4, L'S'J'M') | 1/r_{12} | \phi(n_1l_1, n_2l_2, LSJM) \rangle
$$

= $\tau(-1)^{L+1} \left(\sum_K \left[R_K(1, 2, 3, 4) \langle l_3 || C^K || l_1 \rangle \langle l_4 || C^K || l_2 \rangle \left(\frac{l_3}{l_2} \frac{l_4}{l_1} \frac{L}{K} \right) \right.\right)$
+ $(-1)^{L+S} R_K(2, 1, 3, 4) \langle l_3 || C^K || l_2 \rangle \langle l_4 || C^K || l_1 \rangle \left(\frac{l_3}{l_1} \frac{l_4}{l_2} \frac{L}{K} \right) \delta_{\mathbf{M} \mathbf{M}'} \delta_{SS'} \delta_{LL'} \delta_{JJ'},$ (4a)

and

where

 $\langle l \Vert C^K \Vert l' \rangle = (-1)^l [(2l+1)(2l'+1)]^{1/2} \begin{pmatrix} l' & K & l' \\ 0 & 0 & 0 \end{pmatrix}$ (4b)

$$
R_K(1, 2, 3, 4) \equiv \int_0^\infty \int_0^\infty P_{n_1 l_1}(i) P_{n_2 l_2}(j) \langle r \rangle_K^{K+1}
$$

$$
\times P_{n_3 l_3}(i) P_{B l_4}(j) dr_i dr_j. \quad (4c)
$$

TABLE I. X-ray and Auger energy shifts in eV from the normal configuration^a of neon $(1s¹2s²2p⁶)$, calculated with the adiabatic method, for various configurations of neon $\left(1s^l 2s^m 2p^n\right)$

Configuration			ΔE_x	ΔE_A	ΔE_A	ΔE_A	
ı	\boldsymbol{m}	\pmb{n}	$(2p+1s)$	$(2s - 2s)$	$(2s-2p)$	$(2p-2p)$	
1	$\mathbf 2$	6	0.0	0.0	0.0	0.0	
$\mathbf{1}$	$\bf{2}$	5	5.2	-15.2	-17.2	-19.5	
$\mathbf{1}$	$\boldsymbol{2}$	$\overline{\mathbf{4}}$	12.2	-30.4	-35.1	-40.4	
$\mathbf{1}$	$\bf 2$	3	20.5	-45.7	-53.8	-62.7	
$\mathbf{1}$	$\bf{2}$	$\bf{2}$	30.5	-60.9	-73.0	-86.3	
$\mathbf{1}$	$\bf 2$	$\mathbf{1}$	42.2	-75.7	-92.6	\cdots	
$\mathbf{1}$	$\mathbf{1}$	6	6.1		-19.4	-16.3	
$\mathbf{1}$	$\mathbf{1}$	5	12.4		-37.4	-37.0	
$\mathbf{1}$	$\mathbf{1}$	4	20.4		-56.2	-59.1	
$\mathbf{1}$	$\mathbf{1}$	3	30.0		-75.5	-82.5	
$\mathbf{1}$	$\mathbf 1$	$\bf{2}$	41.2		-95.2	-106.9	
$\mathbf{1}$	$\mathbf{1}$	$\mathbf{1}$	54.1		-116.4	.	
$\mathbf{1}$	$\mathbf 0$	6	13.2			-33.6	
$\mathbf{1}$	$\mathbf 0$	5	20.7			-55.5	
$\mathbf{1}$	$\bf{0}$	$\overline{\mathbf{4}}$	29.8			-78.5	
$\mathbf{1}$	$\bf{0}$	3	40.5			-102.8	
$\mathbf{1}$	$\bf{0}$	$\bf 2$	53.1			-129.2	
$\mathbf{1}$	$\mathbf 0$	$\mathbf{1}$	65.9			.	
$\bf{0}$	$\overline{\mathbf{2}}$	$\boldsymbol{6}$	96.9	68.6	67.3	65.4	
$\bf{0}$	$\overline{\mathbf{2}}$	5	103.8	52.6	48.3	42.9	
$\bf{0}$	$\bf 2$	4	112.2	36.7	28.5	19.0	
0	$\overline{\mathbf{2}}$	$\bf 3$	122.2	20.8	8.1	-6.2	
0	$\overline{\mathbf{2}}$	$\bf 2$	133.8	5.0	-12.9	-32.7	
$\bf{0}$	$\overline{2}$	$\mathbf{1}$	146.8	-10.6	-34.5	\ddotsc	
$\bf{0}$	$\mathbf{1}$	$\bf 6$	103.9		45.8	46.5	
0	$\mathbf{1}$	5	111.9		25.9	22.8	
$\bf{0}$	$\mathbf{1}$	$\overline{\mathbf{4}}$	121.4		5.3	-2.3	
$\pmb{0}$	$\mathbf 1$	$\mathbf{3}$	132.4		-15.8	-28.6	
0	$\mathbf{1}$	$\bf{2}$	145.0		-37.4	-56.2	
$\pmb{0}$	$\mathbf{1}$	$\mathbf 1$	159.1		-59.8	\ddotsc	
$\bf{0}$	$\bf{0}$	$\bf 6$	111.8		.	26.5	
$\mathbf 0$	$\mathbf 0$	5	120.8			1.7	
0	$\bf{0}$	$\overline{\mathbf{4}}$	131.4			-24.4	
0	$\bf{0}$	3	143.5			-51.7	
$\bf{0}$	$\mathbf 0$	$\overline{\mathbf{2}}$	164.0			-80.5	

 $E_{\mathbf{x}}(2p \rightarrow 1s) = 848.5 \text{ eV}; E_{\mathbf{A}}(2s-2s) = 747.3 \text{ eV}; E_{\mathbf{A}}(2s-2p) = 780.0 \text{ eV}; E_{\mathbf{A}}(2p-2p) = 807.7 \text{ eV}.$

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The standard notation of $3-j$ and $6-j$ symbols⁴³ is used in (4a). We have $\tau = \sqrt{\frac{1}{2}}$ if $n_1 l_1$ and $n_2 l_2$ are equivalent electrons; otherwise $\tau=1$. The Auger group rate now can be expressed as

$$
T_A(n_3l_3 - n_1l_1, n_2l_2) = \pi N_{12} \sum_{J} \frac{2J+1}{2l_3+1} \sum_{l_4} |\mathfrak{M}|^2 , \qquad (5)
$$

with M given by Eqs. (4). The total Auger rate Γ_A is the sum of the all possible Auger groups as defined in Eq. (5).

Similarly, the total x-ray rate Γ_x for filling a single vacancy will be the sum of all possible individual transitions, which are given in the electric dipole approximation as

$$
T_x = \frac{4}{3} k^3 \frac{l}{2l_3 + 1} \left| \int_0^\infty P_{n_f l_f} P_{n_3 l_3} r \, dr \right|^2. \tag{6}
$$

The value of k is equal to the x-ray transition energy divided by c . The above rate is reduced by the ratio of the actual number of electrons in the n_tl_t orbital to the maximum possible number of electrons this orbital can have, $(4l, +2)$.

C. Transition Energies

The x-ray transition energies and the Augerelectron energies of the initial configurations $(1s¹2s^m2pⁿ)$ of neon were calculated by computing the appropriate differences of the total energy of the atom in the initial state and in the final state:

$$
E_x(2p + 1s) = E_T(1s^1 2s^m 2p^n) - E_T(1s^{1+1} 2s^m 2p^{n-1}),
$$

\n
$$
E_A(1s-2s-2s) = E_T(1s^1 2s^m 2p^n)
$$

\n
$$
- E_T(1s^{1+1} 2s^{m-2} 2p^n),
$$

\n
$$
E_A(1s-2s-2p) = E_T(1s^1 2s^m 2p^n)
$$

\n
$$
- E_T(1s^{1+1} 2s^{m-1} 2p^{n-1}),
$$

\n
$$
E_A(1s-2p-2p) = E_T(1s^1 2s^m 2p^n)
$$

\n
$$
- E_T(1s^{1+1} 2s^m 2p^{n-2}).
$$

The total energy of the atom in rydbergs for the electronic configuration $1s^{i}2s^{m}sb^{n}$ is given by Slater⁴² in terms of I 's (average kinetic energy and average electron-nucleus interaction energy) and the electrostatic integrals, F^* and G^* :

$$
E_T = U(1s) + mI(2s) + nI(2p) + \frac{1}{2}l(l-1)F^0(1s,1s) + \frac{1}{2}m(m-1)F^0(2s,2s) + \frac{1}{2}n(n-1)[F^0(2p,2p) - \frac{2}{25}F^2(2p,2p)] + lm[F^0(1s,2s) - \frac{1}{2}G^0(1s,2s)] + ln[F^0(1s,2p) - \frac{1}{6}G^1(1s,2p)] + mn[F^0(2s,2p) - \frac{1}{6}G^1(2s,2p)].
$$

The occupation numbers for orbitals 1s, 2s, and 2p are denoted by l, m, and n, respectively.

All quantities appearing in the above equation were calculated with the HFS wave functions discussed in Sec. IIA for neon.

TABLE H. Single-hole K-shell Auger rates, x-ray rates, and fluorescence yields for various configurations of neon $(1s^12s^m2p^n)$.

Configuration		$2s-2s$	$2s - 2p$	$2p - 2p$	Total Auger rate	Total x-ray rate	
\pmb{n}	m	$(10^{-4}a.u.)$	$(10^{-4}a.u.)$	$(10^{-4}a.u.)$	$(10^{-4}a.u.)$	$(10^{-4}a.u.)$	$\omega_{\mathbf{K}}$
6	$\boldsymbol{2}$	8.334	24.448	55.284	88.066	1.436	0.0160
5	$\mathbf 2$	9.393	24.002	45.358	78.753	1.339	0.0167
4	$\overline{2}$	10.701	22.507	33.070	66.278	1.194	0.0177
3	$\boldsymbol{2}$	12.220	19.682	19.731	51.633	0.994	0.0189
$\bf 2$	$\overline{\mathbf{2}}$	13.827	15.163	7.698	36.687	0.732	0.0196
1	$\overline{2}$	15.388	8.606	\cdots	23.994	0.401	0.0164
6	1	\cdots	14.150	66.278	80.428	1.596	0.0195
5	$\mathbf{1}$		13.773	53.548	67.321	1.479	0.0215
4	1		12.832	38.330	51.162	1.312	0.0250
3	1	.	11.129	22.495	33.624	1.087	0.0313
$\boldsymbol{2}$	1		8.442	8.670	17.113	0.796	0.0445
$\mathbf{1}$	$\mathbf{1}$	\cdots	4.716	\ddotsc	4.716	0.434	0.0843
6	$\mathbf 0$.	\cdots	77.901	77.901	1.762	0.0221
5	Ω	.	.	61.854	61.854	1.625	0.0256
4	$\bf{0}$.	\cdots	43.571	43.571	1.435	0.0319
3	$\mathbf 0$		\cdots	25.306	25.306	1.183	0.0447
$\overline{2}$	$\bf{0}$		\cdots	9.682	9.682	0.868	0.0823
1	$\bf{0}$	\cdots	\ddotsc	\cdots	\cdots	0.509	\cdots

III. NUMERICAL RESULTS

Numerical results are presented for all configurations $(1s)'(2s)''(2p)''$ of neon where $l=0, 1$ and $m+n > 0$. The energy shifts from the "normal" configuration are listed in Table I. The calculated individual Auger rates, $2p + 1s$ x-ray rates, and K-shell fluorescence yields are given in Table II for a single K -shell vacancy in Table III for double K-shell vacancies. Auger matrix elements, which can be used in interpreting⁴⁴⁻⁴⁷ the highresolution experimental data on the relative Auger-electron intensities, are given in Table IV.

IV. COMPARISONS

A. Comparison with Statistical Scaling Procedure

Larkins has proposed a simple approximate statistical scaling procedure to obtain the fluorescence yields for multiply ionized atoms when the theoretical x-ray and Auger rates are available for atoms with only one inner-shell vacancy. The for atoms with only one inner-shell vacancy. The technique, used by Larkins³⁷ and Fortner *et al.*,³⁸ is to scale the individual Auger group rates and the x-ray rates, calculated for a single inner-shell vacancy, with the weighting factors $[N_{ij}]$ in Eq. (3)] which depend upon the number of electrons in each subshell. The fluorescence yields can then be calculated for different defect configurations. This simple procedure neglects the effects on the x-ray and Auger transition energies and

the wave functions which result from the multiply ionized configurations.

We present in Fig. 1 the percentage deviation in the x-ray $(2p+1s)$ rate of this approximate model from our HFS calculations. The use of the same x-ray matrix element M_0 in the statistical scaling procedure for all defect electronic configurations introduces the most serious error in the x-ray rate. This is illustrated in Fig. 2, where the ratio of $|M|^2$ and $|M_0|^2$ is plotted for various defect configurations. The matrix element M was calculated for each configuration by using the converged HFS wave functions. Figure 3 contains the percentage deviation in the total Auger rate Γ_A , computed with the statistical scaling procedure from our explicit HFS calculations. Similar comparisons of the K -shell fluorescence yield for configurations with single and double K vacancies are presented in Fig. 4 and Fig. 5, respectively.

Large errors are evidently introduced by the statistical approximation for most electronic configurations of neon.

8. Comparison with Experiments

The experimental value⁴⁸ of the K -shell fluorescence yield for the electronic configuration $(1s)^{1}(2s)^{2}(2p)^{6}$ is 0.018 \pm 0.04, which is to be compared with our calculated value of 0.016. Detailed calculations⁴⁹ including the configuration
interaction^{50,51} between final states of the same $\rm interaction^{50,51}$ between final states of the same

TABLE III. Double-hole K-shell Auger rates, x-ray rates, and fluorescence yields for various configurations of neon $(1s^0 2s^m 2p^n)$.

	Configuration	$2s-2s$	$2s-2p$	$2p - 2p$	Total Auger rate	Total x-ray rate	
n	\boldsymbol{m}	$(2 \times 10)^{-4}$ a.u.)	$(2 \times 10^{-4} a.u.)$	$(2 \times 10^{-4} a.u.)$	$(2 \times 10^{-4} a.u.)$	$(2 \times 10^{-4} a.u.)$	$\omega_{\bm K}$
6	$\bf 2$	10.239	33.699	85.925	129.860	2.363	0.0179
5	$\bf{2}$	11.698	32.558	67.900	112.160	2.162	0.0189
$\boldsymbol{4}$	$\bf{2}$	13.390	30.020	47.598	91.009	1.893	0.0204
$\bf 3$	$\overline{\mathbf{2}}$	15.246	25.753	27.310	68.309	1.547	0.0221
$\bf{2}$	$\overline{\mathbf{2}}$	17.160	19.398	10.233	46.790	1.117	0.0233
1	$\bf 2$	18.930	10.772	\cdots	29.702	0.599	0.0198
6	1	\cdots	19.192	99.936	119.128	2.611	0.0214
5	1	\cdots	18.446	78.032	96.478	2.381	0.0241
$\overline{\mathbf{4}}$	$\mathbf{1}$	\bullet \bullet \bullet	16.928	54.054	70.982	2.078	0.0284
3	1	\cdots	14.415	30.757	45.172	1.693	0.0361
$\boldsymbol{2}$	$\mathbf{1}$	\bullet \bullet \bullet	10.726	11.475	22.201	1.219	0.0520
$\mathbf{1}$	$\mathbf{1}$	\bullet \bullet \bullet	5.872	\cdots	5.872	0.651	0.0998
6	$\mathbf 0$	\cdots	\cdots	116.220	116.220	2.936	0.0246
5	$\bf{0}$	\bullet \bullet	0.0.0	89.805	89.805	2.675	0.0289
4	$\bf{0}$	0 0 0	$\bullet\bullet\bullet$	61.849	61.849	2.336	0.0364
3	$\mathbf 0$	\cdots	\bullet \bullet \bullet	35.184	35.184	1.907	0.0514
$\boldsymbol{2}$	$\mathbf 0$	\bullet \circ \circ	\cdots	13.161	13.161	1.415	0.0971
$\mathbf 1$	$\bf{0}$	\cdots	\cdots	\cdots	\cdots	0.758	.

ı	Configuration \boldsymbol{m}	$\pmb n$	$R_0(20, 20, 10, k0)$	$R_0(20, 21, 10, k1)$	$R_1(21, 20, 10, k1)$	$R_1(21, 21, 10, k0)$	$R_1(21, 21, 10, k2)$
1	$\boldsymbol{2}$	$\boldsymbol{6}$	1.1517	0.9299	1.3948	-1.3677	3.5019
$\mathbf{1}$	$\overline{\mathbf{2}}$	5	1.2227	1.0093	1.5225	-1.5232	3.8836
$\mathbf{1}$	$\overline{2}$	4	1.3050	1.0927	1.6611	-1.6861	4.2797
1	$\mathbf 2$	3	1.3946	1.1798	1.8112	-1.8552	4.6724
1	$\overline{2}$	$\overline{2}$	1.4834	1.2681	1.9693	-2.0221	5.0517
$\mathbf{1}$	$\overline{\mathbf{2}}$	$\mathbf{1}$	1.5649	1.3508	2.1259	$\ddot{}\bullet\dot{}\bullet$	\cdots
$\mathbf{1}$	$\bf{2}$	$\pmb{0}$	1.6329	\bullet .	\cdots	\cdots	\ddotsc
1	$\mathbf{1}$	$\bf{6}$	\cdots	1.0004	1.50612	-1.5013	3.8335
$\mathbf{1}$	$\mathbf{1}$	5	\cdots	1.0812	1.6399	-1.6591	4.2189
1	$\mathbf{1}$	$\overline{4}$	\cdots	1.1668	1.7866	-1.8253	4.6055
1	$\mathbf{1}$	3	\cdots	1.2546	1.9443	-1.9911	4.9869
1	1	$\mathbf 2$	\cdots	1.3379	2.1039	-2.1468	5.3611
$\mathbf{1}$	$\mathbf{1}$	$\mathbf{1}$	\cdots	1.4137	2.2586	\ddotsc	\cdots
1	$\bf{0}$	66	$\ddot{}$	\cdots	\ddotsc	-1.6312	4.1554
1	$\pmb{0}$	5	\cdots	\ddotsc	\cdots	-1.7930	4.5324
1	$\bf{0}$	$\overline{\bf 4}$	\cdots	\cdots	\ddotsc	-1.9547	4.9086
1	0	3	\cdots	\ddotsc	\cdots	-2.1091	5.2899
1	$\bf{0}$	$\bf{2}$	\cdots	\ddotsc	\cdots	-2.2717	5.6649
0	$\boldsymbol{2}$	$\boldsymbol{6}$	1.2765	1.0905	1.7721	-1.7198	4.3628
0	$\bf{2}$	5	1.3645	1.1740	1.9160	-1.8768	4.7491
0	$\boldsymbol{2}$	$\boldsymbol{4}$	1.4598	1.2602	2.0666	-2.0383	5.1313
$\mathbf{0}$	$\bf 2$	$\bf{3}$	1.5577	1.3475	2.2205	-2.1971	5.4941
0	$\bf 2$	$\bf 2$	1.6526	1.4321	2.3686	-2.3407	5.8228
0	$\bf{2}$	$\mathbf{1}$	1.7357	1.5091	2.5025	\cdots	\ddotsc
0	$\boldsymbol{2}$	$\bf{0}$	1.8325	\ddotsc	\ddotsc	$\bullet\bullet\bullet$	\ddotsc
0	$\mathbf{1}$	6	\cdots	1.1632	1.9192	-1.8569	4.7047
0	$\mathbf{1}$	$\overline{\mathbf{5}}$	\cdots	1.2490	2.0717	-2.0198	5.0895
0	$\mathbf{1}$	$\overline{\mathbf{4}}$	\cdots	1.3373	2.2321	-2.1843	5.4659
0	$\mathbf{1}$	3	\cdots	1.4246	2.3939	-2.3405	5.8288
0	1	$\boldsymbol{2}$	\bullet \bullet \bullet	1.5047	2.5437	-2.4789	6.1660
$\bf{0}$	$\mathbf{1}$	$\mathbf{1}$	\cdots	1.5743	2.6644	\ddotsc	$\ddot{}$
0	$\bf{0}$	$\bf 6$	\cdots	\ddotsc	\cdots	-2.0101	5.0719
0	$\mathbf 0$	5	\ddotsc	\ddotsc	\ddotsc	-2.1778	5.4578
0	0	4	\cdots	\cdots	\cdots	-2.3413	5.8457
0	$\bf{0}$	3	.	\cdots	\ddotsc	-2.4992	6.2350
0	0	$\overline{2}$	\ddotsc	\ddotsc	\bullet \bullet \bullet	-2.6625	6.6020

TABLE IV. Auger radial matrix elements for various configurations of neon $(1s^12s^m2p^n)$. The tabulated values of matrix elements are to be multiplied by 10^{-2} .

symmetry agree reasonably well with the highresolution data of Auger-electron energies
and relative intensities.⁴⁶ and relative intensities.

As mentioned earlier K-shell vacancies produced in heavy-ion-atom collisions are usually accompanied by multiple inner-shell ionization. This is in contrast to proton-atom or electron
atom collisions. Burch $et al.^{29}$ have measured atom collisions. Burch $et~al.^{29}$ have measure the ratios of the yields for 30-MeV oxygen-neon and 5-MeV proton-neon collisions. A relative fluorescence yield, ω_{K} (oxygen)/ ω_{K} (proton) = 2.4 $± 0.5$, was found. Their low-resolution measurements also included x-ray transition energies $(2p-1s)$ and Auger-electron energies. The

population of the various defect configurations of neon produced in oxygen-neon collisions cannot be inferred from a comparison of the theoretical energy shifts in the low-resolution theoretical energy shifts in the low-resolution
experimental data.⁵² However, the configuration $(1s)^{1}(2s)^{1}(2p)^{n}$ with $n = 2$ and 3, and $(1s)^{1}(2s)^{0}(2p)^{n}$ with $n = 3$ and 4, are consistent with the relative fluorescence yield and the observed shifts in the x-ray and Auger transition energies. The relative population of the defect configurations cannot be ascertained until high-energy resolution data for the x-rays and the Auger electrons become available. Such experiments are being planned at several laboratories.

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