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Theoretical K-Shell Fluorescence Yield of Multiply Ionized Neon*

C. P. Bhalla and M. Hein
Kansas State University, Department of Physics, Manhattan, Kansas 66506
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The K-shell fluorescence yield has been calculated with the Hartree-Fock-Slater model for all multiply ionized states of neon. These results are compared with the recently measured average K-shell fluorescence yield for 30-MeV O^{7+} collisions with Ne. It is also shown that the commonly used statistical scaling procedure leads to significant errors for neon.

Several authors have reported the shifts of the x-ray transition energies[1-5] and the Auger-electron energies[6] when an inner-shell vacancy is produced in heavy-ion–atom collisions. These energy shifts result from the additional degree of ionization of the atom when an inner-shell vacancy is produced. The x-ray rates, Auger rates, and thus the fluorescence yield ω_K are also affected by the charge state and the configuration of the atom before de-excitation occurs. Since multiple-ionization states are dominantly found in heavy-ion–atom collisions, it is essential to know the variation of ω_K with charge state and electronic configuration. An approximate procedure (statistical scaling) for calculating these fluorescence yields is that proposed by Larkins[7] and employed by Fortner *et al.*[8]

It is the purpose of this Letter to present a consistent analysis of the experimental data for 30-MeV oxygen-neon collisions, as recently observed by Burch *et al.*,[9] and to show that the statistical scaling procedure[7] leads to significant errors in ω_K for low Z.

The K-shell fluorescence yield is defined as

$$\omega_K = T_X/(T_X + T_A),$$

where T_X and T_A are respectively the total x-ray rate and the total Auger rate. The Hartree-Fock-Slater (HFS) atomic model, with the exchange approximation of Herman, Van Dyke, and Ortenburger, was employed in the present calculations.[10] The bound-state wave functions were calculated with the self-consistent HFS model for every possible configuration of neon: $(1s)^l(2s)^m(2p)^n$ with $l = 0, 1, 2$, $m = 0, 1, 2$, and $n = 6$ to 1. The x-ray and the Auger-electron energies were computed by the differences of the total energies of the appropriate electronic configurations.[11] The Auger matrix elements were computed numerically with the relevant bound-state and the continuum-state wave functions. The total Auger rate T_A, which is independent of the choice of the coupling schemes, was obtained by adding the individual Auger group rates. T_X was calculated with the HFS wave functions appropriate for each configuration. The values of ω_K were obtained from T_X and T_A for all the thirty different electronic configurations. The solid lines in Fig. 1 give the results of our calculations.

An estimate of the accuracy of our HFS calculations can be obtained by the following observations: For the $(1s)^1(2s)^2(2p)^6$ configuration of neon, our theoretical ω_K of 0.016 is to be compared with the experimental value[12] of 0.018 $\pm$ 0.004. The deviations of our x-ray transition energies from the Hartree-Fock results are $\approx 0.04\%$ and $\approx 0.01\%$, respectively, for the single K-vancancy and the double K-vacancy configura-

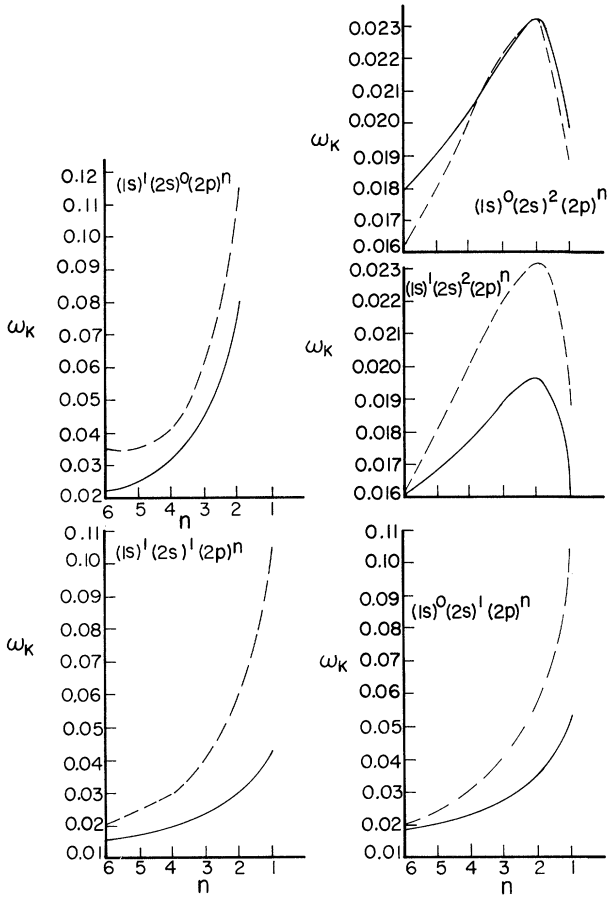

FIG. 1. Theoretical K-shell fluorescence yield ω_K versus the number of electrons in the $2p$ shell for various electronic configurations of neon. The solid lines represent the results of our explicit calculations with the Hartree-Fock-Slater model for each configuration. The corresponding values obtained with an approximate statistical scaling procedure, as commonly used (Ref. 7), are shown as dashed lines. The calculations refer only to the positive-integer values of n, and the lines are drawn simply to guide the eye.

tions. Another meaningful comparison is of the total Auger rates calculated with the HFS model, and the most sophisticated theoretical Auger rate reported by Chase, Kelly, and Köhler,[13] who include the correlation effects. Our value of $T_A = 0.008\,81$ a.u.$^{-1}$ is to be compared with a value of $0.008\,97$ a.u.$^{-1}$ for the $(1s)^1(2s)^6$ configuration. Similar comparisons of T_A cannot be presented for other electronic configurations since the theoretical results with the inclusion of the many-body effects are not available. It may be reasonable to assume $\approx 5\%$ uncertainty in the absolute values of our calculated K-shell fluorescence yields for neon.

Burch *et al.*[9] have measured the Auger-electron energies, K-x-ray energies, and the ratio of yields for both 5-MeV protons and 30-MeV oxygen on neon. X-ray and Auger-electron energy shifts were obtained as well as the ratio of the fluorescence yields, $\omega_K(\mathrm{O})/\omega_K(\mathrm{proton}) = 2.4 \pm 0.5$. The K-shell fluorescence yield, $\omega_K(\mathrm{proton}) \equiv \omega_0$, for the vacancy produced by proton bombardment corresponds predominantly to the $(1s)^1(2s)^2(2p)^6$ configuration. The deviation of the ω_K/ω_0 ratio from unity is an indication of the additional electron stripping when the K-shell vacancy is produced by the oxygen ions. Most experiments, as the one described above, which measure x-ray and Auger-electron yields, are not performed with sufficient resolution to observe all the various configurations populated in the ion-atom collision. The fluorescence yield that one measures in this type of experiment is a weighted average of the appropriate fluorescence yields, as calculated in this paper. The measured fluorescence yield in this type of experiment therefore can vary with the energy of the incident ion, since the collisions at different energies populate different sets of states. The most probable configuration may be determined by comparing the measured and the calculated energy shifts.

The theoretical results for pure configurations, which give ω_K/ω_0 consistent with the measured value of Burch *et al.*, are presented in Table I. The theoretical values of the x-ray energy shifts, ΔE_x, and the Auger-electron energy shifts, ΔE_A, are given in the last three columns. The experimental values of ΔE_x rule out the configurations with double-K vacancies. The broad, unresolved Auger-electron spectrum, as observed by Burch *et al.*, seems to favor the electronic configurations $(1s)^1(2s)^1(2p)^2$, $(1s)^1(2s)^0(2p)^4$, and $(1s)^1(2s)^0(2p)^3$. A more detailed analysis cannot be performed till high-resolution experimental data become available.

It is of interest also to compare the theoretical values of ω_K calculated *explicitly* with the HFS model for each configuration with the values obtained with a simple statistical scaling method.[7] The procedure in this approximate statistical model is to *scale* the individual Auger and x-ray rates, calculated *only* for the $(1s)^1(2s)^2(2p)^6$ configuration, with the weighting factors, which depend upon the actual number of electrons in a shell for *other* configurations. The approximations are, then, the ignoring of the changes in the wave functions and the transition energies because of the additional vacancies in the $2s$ and

TABLE I. Theoretical ratios of the K-shell fluorescence yield ω_K and the normal K-shell fluorescence ω_0 for various configurations of neon $(1s)^1(2s)^m(2p)^n$, the theoretical x-ray energy shifts, and the calculated Auger-electron energy shifts.

Configuration			$\frac{\omega_K}{\omega_0}$	ΔE_X (eV)	$\Delta E_A(1s\text{-}2p\text{-}2p)$ (eV)	$\Delta E_A(1s\text{-}2s\text{-}2p)$ (eV)
l	m	n	HFS[a]	HFS	HFS	HFS
1	1	2	1.9	41	−107	−95
1	1	1	2.7	54	...	−116
1	0	4	2.0	30	−79	...
1	0	3	2.8	41	−103	...
0	1	2	2.2	145	−56	−37
0	0	4	2.3	131	−24	...

[a] $\omega_0 = 0.016$ for the $(1s)^1(2s)^2(2p)^6$ configuration.

the $2p$ shells.

The dashed lines in Fig. 1 represent the values of ω_K using the statistical model for neon. This approximate procedure introduces errors as much as 25 to 139% for the $(1s)^1(2s)^1(2p)^n$ configurations and 12 to 100% for the $(1s)^0(2s)^1(2p)^n$ configurations. The range of the erros in the statistical model is 0 to 18% and 15–40% for the configurations $(1s)^1(2s)^2(2p)^n$ and $(1s)^1(2s)^0(2p)^n$, respectively.

In conclusion, the explicit HFS calculations of the K-shell fluorescence yield for different charge states and electronic configurations of neon are presented here and are found to be essential to the correct interpretation of the ionization of neon by heavy ions. Also the statistical scaling procedure for defect configurations is shown to lead to serious errors in calculating ω_K for low Z and should, therefore, be used with caution.

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