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Theoretical fluorescence yields for neon*

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Theoretical expressions for the Auger rates of various spectroscopic terms of electronic configurations $1s^1 2s^2 2p^n$, $1s^1 2s^0 2p^n$, and $1s^1 2s^1 2p^n$ ($n = 6 \rightarrow 1$) are presented. Numerical values of the x-ray transition energies and the multiplet partial fluorescence yields are given for variously ionized neon.

I. INTRODUCTION

The deexcitation of an atom with an inner-shell vacancy can occur mainly by two independent processes: (a) the emission of x rays and (b) the ejection of Auger electrons. There are only a few calculations relevant for multiply-ionized atoms.[1,2] In these calculations the average x-ray and Auger rates, $\overline{\Gamma}_x$ and $\overline{T}_A$, were calculated for various electronic configurations. The theoretical formulas used in these calculations correspond to performing averages of the x-ray (and Auger) rates for spectroscopic terms of a configuration with a statistical population. If N represents the number of atoms with a particular electronic configuration and N_x denotes the number of atoms which decay by x-ray transitions, then a mean theoretical fluorescence yield, $\overline{\omega}$, was defined as follows:

$$\frac{N_x}{N} \equiv \frac{\overline{\Gamma}_x}{\overline{\Gamma}_x + \overline{T}_A} = \overline{\omega} \ . \tag{1}$$

A brief discussion concerning the inadequacy of the above definition was presented earlier.[3,4] We review first some of the relevant definitions.

Consider an electronic configuration with an arbitrary number of open shells. Let us designate by quantum numbers $\alpha_i J_i$ and $\alpha_f J_f$, respectively, one of the initial-state levels and the resulting final state after the x-ray emission. The number of atoms, which will decay by the $\alpha_i J_i \rightarrow \alpha_f J_f$ x-ray transition, $N_x(\alpha_i J_i \rightarrow \alpha_f J_f)$, can be represented in terms of the x-ray width, $\Gamma_x(\alpha_i J_i \rightarrow \alpha_f J_f)$, the total width of the initial level, $\Gamma(\alpha_i J_i)$, and the number of atoms in the initial state at time $t=0$, $N(\alpha_i J_i)$:

$$\begin{aligned} N_x(\alpha_i J_i \rightarrow \alpha_f J_f) &= \int_0^\infty dt\, N(\alpha_i J_i)\Gamma_x(\alpha_i J_i \rightarrow \alpha_f J_f) \\ &\quad \times \exp[-\Gamma(\alpha_i J_i)t] \\ &= N(\alpha_i J_i)\Gamma_x(\alpha_i J_i \rightarrow \alpha_f J_f)/\Gamma(\alpha_i J_i). \end{aligned}$$

The line fluorescence yield is, therefore, given by

$$\begin{aligned} \omega(\alpha_i J_i \rightarrow \alpha_f J_f) &= \frac{N_x(\alpha_i J_i \rightarrow \alpha_f J_f)}{N(\alpha_i J_i)} \\ &= \frac{\Gamma_x(\alpha_i J_i \rightarrow \alpha_f J_f)}{\Gamma(\alpha_i J_i)} \ . \end{aligned} \tag{2}$$

If no distinction is to be made between the various lines originating from a certain initial level, it is convenient to define the level fluorescence yield

$$\begin{aligned} \omega(\alpha_i J_i) &= \frac{\sum_{J_f} N_x(\alpha_i J_i \rightarrow \alpha_f J_f)}{N(\alpha_i J_i)} \\ &= \sum_{J_f} \omega(\alpha_i J_i \rightarrow \alpha_f J_f). \end{aligned} \tag{3}$$

The multiplet partial fluorescence yields relevant for a transition between two multiplets can be defined as follows (if the spin-orbit coupling can be neglected as compared to the electrostatic interactions):

$$\omega(\alpha_i S_i L_i \rightarrow \alpha_f S_f L_f) = \frac{\sum_i (2J_i+1)\omega(\alpha_i S_i L_i J_i)}{\sum_i (2J_i+1)} \ . \tag{4a}$$

We can rewrite Eq. (4a) in the cases when both the x-ray and Auger transitions are allowed:

$$\begin{aligned} \omega(\alpha_i S_i L_i \rightarrow \alpha_f S_i L_f) \\ = \Gamma_x(\alpha_i S_i L_i \rightarrow \alpha_f S_i L_f)/\Gamma(\alpha_i S_i L_i). \end{aligned} \tag{4b}$$

It may still be convenient and in some cases desirable to define an effective fluorescence yield for an electronic configuration, for example, for the analyses of spectral measurements where in the lines or the multiplets cannot be resolved:

$$\omega(\text{effective}) \equiv \frac{\sum_i F(\alpha_i J_i)\omega(\alpha_i J_i)}{\sum_i F(\alpha_i J_i)} \ , \tag{5a}$$

where $F(\alpha_i J_i)$ is the relative population of the initial level. If one *assumes*[5] that there is a statistical population of the initial levels for a configuration, we can define average fluorescence yields

$$\langle \omega \rangle = \frac{\sum_i (2J_i+1)\omega(\alpha_i J_i)}{\sum_i (2J_i+1)}$$

$$= \frac{\sum_i (2L_i+1)(2S_i+1)\omega(\alpha_i S_i L_i)}{\sum_i (2L_i+1)(2S_i+1)} . \qquad (5b)$$

It should be noted that $\langle \omega \rangle$ is exactly equal to $\bar{\omega}$ *only when* there is one level for a particular electronic configuration.

In this paper we present theoretical development of the Auger rates for various spectroscopic terms and numerical results concerning the x-ray transition energies between multiplets and their respective multiplet partial fluorescence yields for multiply-ionized neon.

II. THEORY

Atomic units ($\hbar = m_e = e = 1$) are used throughout the following developments.

A. Calculation of Auger rates

Let us designate by quantum numbers $\alpha' S' L' M_{S'} M_{L'}$ the initial state ψ' with an inner-shell vacancy. The final state ψ, which after the Auger transition contains two new vacancies and an electron in the continuum, is specified by quantum numbers $\alpha S L M_S M_L$. If ψ' and ψ are antisymmetrized wave functions, the standard perturbation gives for the Auger rate

$$T_A(i \rightarrow f) = 2\pi\rho_F \overline{\sum} \left| \langle \psi | \sum_{i>j} (1/r_{ij}) | \psi' \rangle \right|^2 .$$

The symbol $\overline{\sum}$ denotes a sum over the final-state magnetic quantum number and the contributions of all the orbital-angular-momentum values of the continuum electron, and an average over the initial-state magnetic quantum numbers. We can choose the normalization of the continuum state so that the density of final state, ρ_F, multiplied by 2π is unity.

The evaluation of the matrix element requires special theoretical techniques, in particular when there is more than one open shell in the initial state. We quote the essential results derived by Fano.[6] Consider the interacting electrons specified by ρ' and σ' (ρ and σ) in the initial (final) state. Note that there are three bound-state orbitals and one continuum-state orbital. All other orbitals are assumed to be occupied by spectator electrons.

The notation of Fano[6] is used below:

$$\langle \psi | \sum_{i>j} (1/r_{ij}) | \psi' \rangle = \tfrac{1}{2}(-1)^{\Delta P}[N_\rho(N_\sigma - \delta_{\rho\sigma})N_{\rho'}(N_{\sigma'} - \delta_{\rho'\sigma'})]^{1/2} \sum_{\epsilon,\epsilon'=0,1} (1-\epsilon\delta_{\rho\sigma})(1-\epsilon'\delta_{\rho'\sigma'})(-1)^{\epsilon-\epsilon'}$$

$$\times \sum (l_\rho^{N_\rho}\alpha_\rho S_\rho L_\rho \llbracket l_\rho^{\bar{N}_\rho - 1}\bar{\alpha}_\rho \bar{S}_\rho \bar{L}_\rho \, l_\rho S_\rho L_\rho)(l_\sigma^{N_\sigma}\alpha_\sigma S_\sigma L_\sigma \llbracket l_\sigma^{\bar{N}_\sigma}\bar{\alpha}_\sigma \bar{S}_\sigma \bar{L}_\sigma \, l_\sigma S_\sigma L_\sigma)$$

$$\times \sum (l_{\rho'}^{N_{\rho'}}\alpha_{\rho'} S_{\rho'} L_{\rho'} \llbracket l_{\rho'}^{\bar{N}_{\rho'}}\bar{\alpha}_{\rho'} \bar{S}_{\rho'} \bar{L}_{\rho'} \, l_{\rho'} S_{\rho'} L_{\rho'})(l_{\sigma'}^{N_{\sigma'}}\alpha_{\sigma'} S_{\sigma'} L_{\sigma'} \llbracket l_{\sigma'}^{\bar{N}_{\sigma'}}\bar{\alpha}_{\sigma'} \bar{S}_{\sigma'} \bar{L}_{\sigma'} \, l_{\sigma'} S_{\sigma'} L_{\sigma'})$$

$$\times (\Phi(\rho\sigma\epsilon, \alpha S) | \Phi'(\rho'\sigma'\epsilon', \alpha' S'))(X(\rho\sigma\epsilon, \alpha L) | (1/r_{N,N-1}) | X'(\rho'\sigma'\epsilon', \alpha' L')) .$$

$N_\rho, N_\sigma, N_{\rho'}$, and $N_{\sigma'}$ are the number of electrons in the shells which are specified by the principal quantum number (n) and orbital quantum number (l) and in particular by $n_\rho l_\rho$, $n_\sigma l_\sigma$, $n_{\rho'} l_{\rho'}$, and $n_{\sigma'} l_{\sigma'}$.

$$(\Phi(\rho\sigma\epsilon, \alpha S) | \phi'(\rho'\sigma'\epsilon', \alpha' S')) = (\bar{S}_1 \cdots \bar{S}_{\rho-1}(\bar{S}_\rho s_{N-1+\epsilon})S_\rho \cdots (\bar{S}_\sigma, s_{N-\epsilon})S_\sigma \cdots, \alpha$$

$$\times | \bar{S}_1 \cdots \bar{S}_{\rho'-1}(\bar{S}_{\rho'} s_{N-1+\epsilon'})S'_{\rho'} \cdots (\bar{S}_{\sigma'} s_{N-\epsilon'})S'_{\sigma'} \cdots, \alpha')^{(S)} \delta_{SS'} ,$$

$$(X(\rho\sigma\epsilon, \alpha L) | (1/r_{N,N-1}) | X'(\rho'\sigma'\epsilon', \alpha' L'))$$

$$= \sum_k \delta_{LL'} \{ \delta_{\epsilon\epsilon'} R^k(n_\rho l_\rho n_\sigma l_\sigma, n_{\rho'} l_{\rho'} n_{\sigma'} l_{\sigma'})[(2l_\sigma+1)(2l_{\rho'}+1)]^{-1/2}(l_\rho \| C^k \| l_{\rho'})(l_\sigma \| C^k \| l_{\sigma'})\Lambda_1$$

$$+ (1-\delta_{\epsilon\epsilon'})R^k(n_\rho l_\rho n_\sigma l_\sigma, n_{\sigma'} l_{\sigma'} n_{\rho'} l_{\rho'})[(2l_\sigma+1)(2l_{\sigma'}+1)]^{-1/2}(l_\rho \| C^k \| l_{\sigma'})(l_\sigma \| C^k \| l_{\rho'})\Lambda_2 \}$$

$$\Lambda_1 \equiv (\bar{L}_1 \cdots \bar{L}_{\rho-1}(\bar{L}_\rho l_\rho)L_\rho \cdots [\bar{L}_\sigma(l_{\sigma'} k)]L_\sigma \cdots, \alpha | \bar{L}_1 \cdots \bar{L}_{\rho'-1}[\bar{L}_{\rho'}(k l_\rho)l_{\rho'}]L_{\rho'} \cdots (\bar{L}_{\sigma'} l_{\sigma'})L_{\sigma'} \cdots, \alpha')^{(L)} ,$$

$$\Lambda_2 = \Lambda_1(\rho' \rightarrow \sigma' \,|\, \sigma' \rightarrow \rho') .$$

The angular-momentum recoupling coefficients[7] are denoted by Λ_1 and Λ_2. The generalized Slater integral R^k contains only the radial functions of the four electrons. Similarly expressions for $\rho = \sigma$ cases are obtained by using Eqs. (26), (35a), and (36a) of Fano's paper.[6] The resulting theoretical expressions for the total Auger rates T_A of the various spectroscopic terms of the $1s^1 2s^2 2p^n$ electronic configurations are listed in Table I. The continuum electron is denoted by

ϵl. The total Auger rates for the terms of $1s^1 2s^1 2p^n$ configuration are defined as sums of T_1 and T_2. The expressions for T_1 are listed in Table II. T_2, whenever it is not zero, is listed below. For the purposes of convenience and brevity, we define the following combinations of generalized Slater integrals and the mixing coefficients, a_{ij}, b_{ij}, and c_{ij}:

$$A_1 \equiv R^0(1s, \epsilon p, 2s, 2p) ,$$

$$A_2 \equiv R^1(1s, \epsilon p, 2p, 2s) - \tfrac{9}{2} R^0(1s, \epsilon p, 2s, 2p) ,$$

$$A_3 \equiv R^1(1s, \epsilon p, 2p, 2s) - \tfrac{3}{2} R^0(1s, \epsilon p, 2s, 2p) ,$$

$$A_4 \equiv R^1(1s, \epsilon p, 2p, 2s) - 4R^0(1s, \epsilon p, 2s, 2p) ,$$

$$A_5 \equiv R^1(1s, \epsilon p, 2p, 2s) - 2R^0(1s, \epsilon p, 2s, 2p) ,$$

$$A_6 \equiv R^1(1s, \epsilon p, 2p, 2s) - \tfrac{9}{4} R^0(1s, \epsilon p, 2s, 2p) ,$$

TABLE I. Theoretical formulas for the total Auger rates for the $1s^1 2s^2 2p^n$ configurations. The coefficients listed below are to be multiplied with terms which are designated by the letters A–F: A is $[R'(1s, \epsilon d, 2p, 2p)]^2$; B, $[R'(1s, \epsilon s, 2p, 2p)]^2$; C, $[R^0(1s, \epsilon s, 2s, 2s)]^2$; D, $[R^0(1s, \epsilon p, 2s, 2p)]^2$; E, $[R^1(1s, \epsilon p, 2p, 2s)]^2$; F, $[R^0(1s, \epsilon p, 2s, 2p)\, R^1(1s, \epsilon p, 2p, 2s)]$.

n	Term	A	B	C	D	E	F
1	^3P	0	0	1	1	0	0
	^1P	0	0	1	1	$\frac{4}{9}$	$-\frac{4}{3}$
2	^4P	0	0	1	2	0	0
	^2D	$\frac{2}{15}$	0	1	2	$\frac{2}{9}$	$-\frac{2}{3}$
	^2P	0	0	1	2	$\frac{2}{3}$	-2
	^2S	0	$\frac{1}{3}$	1	2	$\frac{2}{9}$	$-\frac{2}{3}$
3	^1P	$\frac{1}{9}$	$\frac{2}{9}$	1	3	$\frac{2}{3}$	-2
	^3P	$\frac{1}{9}$	$\frac{2}{9}$	1	3	$\frac{2}{9}$	$-\frac{2}{3}$
	^1D	$\frac{1}{5}$	0	1	3	$\frac{2}{3}$	-2
	^3D	$\frac{1}{5}$	0	1	3	$\frac{2}{9}$	$-\frac{2}{3}$
	^5S	0	0	1	3	0	0
	^3S	0	0	1	3	$\frac{8}{9}$	$-\frac{8}{3}$
4	^2P	$\frac{2}{9}$	$\frac{1}{9}$	1	4	$\frac{8}{9}$	$-\frac{8}{3}$
	^2D	$\frac{16}{45}$	$\frac{1}{9}$	1	4	$\frac{4}{9}$	$-\frac{4}{3}$
	^2S	$\frac{2}{9}$	$\frac{4}{9}$	1	4	$\frac{4}{9}$	$-\frac{4}{3}$
	^4P	$\frac{2}{9}$	$\frac{1}{9}$	1	4	$\frac{2}{9}$	$-\frac{2}{3}$
5	^1P	$\frac{4}{9}$	$\frac{2}{9}$	1	5	$\frac{8}{9}$	$-\frac{8}{3}$
	^3P	$\frac{4}{9}$	$\frac{2}{9}$	1	5	$\frac{4}{9}$	$-\frac{4}{3}$
6	^2S	$\frac{2}{3}$	$\frac{1}{3}$	1	6	$\frac{2}{3}$	-2

TABLE II. Theoretical formulas for the total Auger rates, $T_A = T_1 + T_2$, of the various terms of the $1s2s2p^n$ configurations. To obtain T_1, the coefficients listed below are to be multiplied by terms which are designated by the letters A–E: A is $[R^1(1s, \epsilon d, 2p, 2p)]^2$; B, $[R'(1s, \epsilon s, 2p, 2p)]^2$; C, $[R^0(1s, \epsilon p, 2s, 2p)]^2$; D, $[R'(1s, \epsilon p, 2p, 2s)]^2$; E, $[R^0(1s, \epsilon p, 2s, 2p) R^1(1s, \epsilon p, 2s, 2p)]$.

n	Term	A	B	C	D	E	T_2
6	^1S	$\frac{2}{3}$	$\frac{1}{3}$	3	$\frac{1}{3}$	-2	0
	^3S	$\frac{2}{3}$	$\frac{1}{3}$	0	$\frac{1}{3}$	0	0
5	^4P	$\frac{4}{9}$	$\frac{2}{9}$	0	$\frac{2}{9}$	0	0
	$^2P_+$	$\frac{4}{9}$	$\frac{2}{9}$	…	…	…	[a]
	$^2P_-$	$\frac{4}{9}$	$\frac{2}{9}$	…	…	…	[a]
4	^5P	$\frac{2}{9}$	$\frac{1}{9}$	0	$\frac{1}{9}$	0	0
	^3D	$\frac{16}{45}$	$\frac{1}{9}$	0	$\frac{2}{9}$	0	0
	^1D	$\frac{16}{45}$	$\frac{1}{9}$	8	$\frac{2}{9}$	$-\frac{8}{3}$	0
	^3S	$\frac{2}{9}$	$\frac{4}{9}$	0	$\frac{2}{9}$	0	0
	^1S	$\frac{2}{9}$	$\frac{4}{9}$	8	$\frac{2}{9}$	$-\frac{8}{3}$	0
	^1P	$\frac{2}{9}$	$\frac{1}{9}$	0	$\frac{4}{9}$	0	0
	$^3P_+$	$\frac{2}{9}$	$\frac{1}{9}$	…	…	…	[a]
	$^3P_-$	$\frac{2}{9}$	$\frac{1}{9}$	…	…	…	[a]
3	^4P	$\frac{1}{9}$	$\frac{2}{9}$	0	$\frac{1}{9}$	0	0
	^4D	$\frac{1}{5}$	$\frac{1}{9}$	0	0	0	0
	^2S	0	0	0	$\frac{4}{9}$	0	0
	$^4S_+$	0	0	…	…	…	[a]
	$^4S_-$	0	0	…	…	…	[a]
	$^2D_+$	$\frac{1}{5}$	0	…	…	…	[a]
	$^2D_-$	$\frac{1}{5}$	0	…	…	…	[a]
	$^2P_+$	$\frac{1}{9}$	$\frac{2}{9}$	…	…	…	[a]
	$^2P_-$	$\frac{1}{9}$	$\frac{2}{9}$	…	…	…	[a]
2	^3S	0	$\frac{1}{3}$	0	$\frac{1}{9}$	0	0
	^1S	0	$\frac{1}{3}$	4	$\frac{1}{9}$	$-\frac{2}{3}$	0
	^3D	$\frac{2}{15}$	0	0	$\frac{1}{9}$	0	0
	^1D	$\frac{2}{15}$	0	4	$\frac{1}{9}$	$-\frac{2}{3}$	0
	^1P	$\frac{1}{3}$	0	0	0	0	0
	$^3P_+$	0	0	…	…	…	[a]
	$^3P_-$	0	0	…	…	…	[a]
1	$^2P_+$	0	0	…	…	…	[a]
	$^2P_-$	0	0	…	…	…	[a]

[a] The expressions for T_2 are listed in the text.

$$\phi(1s2s2p^n\ {}^{2Q+1}P_+) = a_{11}\psi(1s2p^n[{}^{2Q+2}P]2s\ {}^{2Q+1}P) + a_{12}\psi(1s2p^n[{}^{2Q}P]2s\ {}^{2Q+1}P),$$

$$\phi(1s2s2p^n\ {}^{2Q+1}P_-) = a_{21}\psi(1s2p^n[{}^{2Q+2}P]2s\ {}^{2Q+1}P) + a_{22}\psi(1s2p^n[{}^{2Q}P]2s\ {}^{2Q+1}P),$$

$$\phi(1s2s2p^3\ {}^4S_+) = b_{11}\psi(1s2p^3[{}^5S]2s\ {}^4S) + b_{12}\psi(1s2p^3[{}^3S]2s\ {}^4S),$$

$$\phi(1s2s2p^3\ {}^4S_-) = b_{21}\psi(1s2p^3[{}^5S]2s\ {}^4S) + b_{22}\psi(1s2p^3[{}^3S]2s\ {}^4S),$$

$$\phi(1s2s2p^3\ {}^2D_+) = c_{11}\psi(1s2p^3[{}^3D]2s\ {}^2D) + c_{12}\psi(1s2p^3[{}^1D]2s\ {}^2D),$$

$$\phi(1s2s2p^3\ {}^2D_-) = c_{21}\psi(1s2p^3[{}^3D]2s\ {}^2D) + c_{22}\psi(1s2p^3[{}^1D]2s\ {}^2D),$$

$$T_2(1s2s2p^5\ {}^2P_+) = \left(\sqrt{\tfrac{2}{9}}\,a_{11}A_2 + \sqrt{\tfrac{3}{2}}\,a_{12}A_1\right)^2 + \left(\sqrt{\tfrac{1}{2}}\,a_{11}A_1 + \sqrt{\tfrac{2}{9}}\,a_{12}A_3\right)^2 + \left(\sqrt{\tfrac{5}{2}}\,a_{11}A_1 + \sqrt{\tfrac{10}{9}}\,a_{12}A_3\right)^2,$$

$$T_2(1s2s2p^5\ {}^2P_-) = \left(\sqrt{\tfrac{2}{9}}\,a_{21}A_2 + \sqrt{\tfrac{3}{2}}\,a_{22}A_1\right)^2 + \left(\sqrt{\tfrac{1}{2}}\,a_{21}A_1 + \sqrt{\tfrac{2}{9}}\,a_{22}A_3\right)^2 + \left(\sqrt{\tfrac{5}{2}}\,a_{21}A_1 + \sqrt{\tfrac{10}{9}}\,a_{22}A_3\right)^2,$$

$$T_2(1s2s2p^4\ {}^3P_+) = \left(\tfrac{1}{3}a_{11}A_4 + \sqrt{\tfrac{8}{9}}\,a_{12}A_1\right)^2 + \left(-\sqrt{\tfrac{4}{3}}\,a_{11}A_1 + \sqrt{\tfrac{1}{6}}\,a_{12}A_5\right)^2 + \left(\sqrt{\tfrac{20}{9}}\,a_{11}A_1 - \sqrt{\tfrac{5}{18}}\,a_{12}A_5\right)^2,$$

$$T_2(1s2s2p^4\ {}^3P_-) = \left(\tfrac{1}{3}a_{21}A_4 + \sqrt{\tfrac{8}{9}}\,a_{22}A_1\right)^2 + \left(-\sqrt{\tfrac{4}{3}}\,a_{21}A_1 + \sqrt{\tfrac{1}{6}}\,a_{22}A_5\right)^2 + \left(\sqrt{\tfrac{20}{9}}\,a_{21}A_1 - \sqrt{\tfrac{5}{18}}\,a_{22}A_5\right)^2,$$

$$T_2(1s2s2p^3\ {}^4S_+) = \left(-\sqrt{\tfrac{15}{4}}\,b_{11}A_1 + \tfrac{2}{3}b_{12}A_6\right)^2,$$

$$T_2(1s2s2p^3\ {}^4S_-) = \left(-\sqrt{\tfrac{15}{4}}\,b_{21}A_1 + \tfrac{2}{3}b_{22}A_6\right)^2,$$

$$T_2(1s2s2p^3\ {}^2D_+) = \left(\tfrac{1}{3}c_{11}A_2 - \sqrt{\tfrac{3}{4}}\,c_{12}A_1\right)^2 + \left(\tfrac{3}{2}c_{11}A_1 - \sqrt{\tfrac{1}{3}}\,c_{21}A_2\right)^2,$$

$$T_2(1s2s2p^3\ {}^2D_-) = \left(\tfrac{1}{3}c_{21}A_2 - \sqrt{\tfrac{3}{4}}\,c_{22}A_1\right)^2 + \left(\tfrac{3}{2}c_{21}A_2 - \sqrt{\tfrac{1}{3}}\,c_{22}A_2\right)^2,$$

$$T_2(1s2s2p^3\ {}^2P_+) = \left(-\tfrac{1}{3}a_{11}A_6 + \sqrt{\tfrac{3}{4}}\,a_{12}A_1\right)^2 + \left(-a_{11}A_1 + \sqrt{\tfrac{4}{27}}\,a_{12}A_3\right)^2 + \left(\sqrt{\tfrac{5}{4}}\,a_{11}A_1 + \sqrt{\tfrac{5}{12}}\,a_{12}A_3\right)^2,$$

$$T_2(1s2s2p^3\ {}^2P_-) = \left(-\tfrac{1}{3}a_{21}A_6 + \sqrt{\tfrac{3}{4}}\,a_{22}A_1\right)^2 + \left(-a_{21}A_1 + \sqrt{\tfrac{4}{27}}\,a_{22}A_3\right)^2 + \left(\sqrt{\tfrac{5}{4}}\,a_{21}A_1 + \sqrt{\tfrac{5}{12}}\,a_{22}A_3\right)^2,$$

$$T_2(1s2s2p^2\ {}^3P_+) = \left(\sqrt{\tfrac{8}{3}}\,a_{11}A_1 - \sqrt{\tfrac{1}{3}}\,a_{12}A_5\right)^2,$$

$$T_2(1s2s2p^2\ {}^3P_-) = \left(\sqrt{\tfrac{8}{3}}\,a_{21}A_1 - \sqrt{\tfrac{1}{3}}\,a_{22}A_5\right)^2,$$

$$T_2(1s2s2p\ {}^2P_+) = \left(-\sqrt{\tfrac{3}{2}}\,a_{11}A_1 + \sqrt{\tfrac{2}{9}}\,a_{12}A_3\right)^2,$$

$$T_2(1s2s2p\ {}^2P_-) = \left(-\sqrt{\tfrac{3}{2}}\,a_{21}A_1 + \sqrt{\tfrac{2}{9}}\,a_{22}A_3\right)^2.$$

Theoretical expressions for the various terms of the $1s^1 2s^0 2p^n$ configuration are obtained from the corresponding formulas for the $1s^1 2s^2 2p^n$ configuration by replacing the following generalized Slater integrals, $R^0(1s, \epsilon s, 2s, 2s)$, $R^0(1s, \epsilon p, 2s, 2p)$, and $R^1(1s, \epsilon p, 2p, 2s)$, by zeros.

B. Calculations of x-ray rates

The theoretical expression for radiative rates, $\Gamma_x(\alpha_i S_i L_i J_i \to \alpha_f S_i L_f J_f)$, are given in standard references.[8-10] Following the notation of Shore and Menzel,[8] we have (in a.u.)

$$\Gamma_x(\alpha_i S_i L_i J_i \to \alpha_f S_f L_f J_f) = \tfrac{4}{3}k^3(2J_i+1)^{-1}\left[R_{\text{line}}(S_i L_f J_f, S_i L_i J_i)R_{\text{mul}}(\alpha_f L_f, \alpha_i L_i)(-1)^{l-l_>}\sqrt{l_>}\,I(nl, n'l')\right]^2$$

where the transition integral,

$$I(nl, n'l') = \int_0^\infty P_{nl}(r)P_{n'l'}(r)r\,dr\,.$$

Similarly, the rate for a transition between multiplets can be written as

$$\Gamma_x(\alpha_i S_i L_i \to \alpha_f S_i L_f) = \tfrac{4}{3}k^3(2L_i+1)^{-1}\left[R_{\text{mul}}(\alpha_f L_f, \alpha_i L_i)(-1)^{l-l_>}\sqrt{l_>}\,I(nl, n'l')\right]^2.$$

III. NUMERICAL RESULTS

The K x-ray transition energies were calculated by computing the differences between the initial-state and the final-state total energies.[11] The explicit expressions are given by Slater[10] in terms of F's and G's. The spin-orbit coupling gives additional energy corrections, which were found to be insignificant (≈0.1 eV) for neon. Therefore, it is sufficient to calculate the multiplet partial fluorescence yields. The generalized Slater integrals needed for the calculations of the Auger rates have been already calculated by Bhalla, Folland, and Hein.[2] Tables III, IV, and V contain the results of our calculations respectively for the $1s^1 2s^2 2p^n$, $1s^1 2s^1 2p^n$, and $1s^1 2s^0 2p^n$ configurations of neon ($n = 1-6$).

Two points concerning the notation and our calculations need further elaboration. Firstly, there is always at least one pair of terms with the *same* values of S and L for the configurations $1s^1 2s^1 2p^n$ ($n = 5 \rightarrow 1$). We have labeled the two terms with a subscript + (−) to indicate that the term has the higher (lower) value of the energy. The wave functions of these terms can be expressed as a linear combination of the two theoretical states with the same S and L values, which can be formed by two different methods of coupling first the $1s$ and the $2p^n$ orbitals and then the $2s$ orbital. For example, consider the two ^2P states of the $1s^1 2s^2 2p^5$ configuration:

$$\Phi(1s2s2p^5\,{}^2P_+) = a_{11}\psi_1 + a_{12}\psi_2\ ,$$

$$\phi(1s2s2p^5\,{}^2P_-) = a_{21}\psi_1 + a_{22}\psi_2\ ,$$

where

$$\psi_1 \equiv \Psi(1s2p^5[{}^3P]2s\ {}^2P)\ ,$$

$$\psi_2 \equiv \Psi(1s2p^5[{}^1P]2s\ {}^2P)\ .$$

The amplitudes $|a_{11}| > |a_{12}|$ and $|a_{22}| > |a_{21}|$. These amplitudes and the eigenvector were calculated by the perturbation theory in this case as well as for other relevant electron configurations. Secondly, there are some terms, for example, $1s^1 2s^1 2p^3\ {}^6S$,

TABLE III. Theoretical x-ray transition energies[a] E_x (in eV) and multiplet partial fluorescence yields, $\omega\,(\alpha L_i S_i \rightarrow \alpha_f L_f S_i)$, for $1s^1 2s^2 2p^n$ configurations of neon.

Initial state	Final state	E_x	$100\omega\,(\alpha L_i S_i \rightarrow \alpha_f L_f S_i)$
$1s2s^22p^1\ {}^1P$	$1s^22s^2\ {}^1S$	895.6	9.57
${}^3P$	···	···	0.0
$1s2s^22p^2\ {}^2D$	$1s^22s^22p\ {}^2P$	881.6	1.45
${}^2P$	${}^2P$	882.9	10.5
${}^2S$	${}^2P$	888.3	1.97
${}^4P$	···		0.0
$1s2s^22p^3\ {}^1P$	$1s^22s^22p^2\ {}^1S$	869.6	1.89
${}^3D$	${}^3P$	869.9	1.07
${}^1D$	${}^1D$	871.3	3.66
${}^3S$	${}^3P$	871.5	6.50
${}^1P$	${}^1D$	875.5	2.36
${}^3P$	${}^3P$	876.9	1.24
${}^5S$	···	···	0.0
$1s2s^22p^4\ {}^2D$	$1s^22s^22p^3\ {}^2P$	859.1	0.39
${}^2P$	${}^2P$	860.0	1.62
${}^4P$	${}^4S$	861.9	0.92
${}^2D$	${}^2D$	862.8	1.16
${}^2P$	${}^2D$	863.6	2.69
${}^2S$	${}^2P$	865.1	1.78
$1s2s^22p^5\ {}^1P$	$1s^22s^22p^4\ {}^1S$	850.4	0.47
${}^3P$	${}^3P$	854.6	1.32
${}^1P$	${}^1D$	855.4	2.33
$1s2s^22p^6\ {}^2S$	$1s^22s^22p^5\ {}^2P$	848.8	1.60

[a] These transition energies are reported by House, (Ref. 11) who used the Hartree-Fock atomic model.

TABLE IV. Theoretical x-ray transition energies[a] E_x (in eV) and multiplet partial fluorescence yields $\omega(\alpha L_i S_i \rightarrow \alpha_f L_f S_i)$ for $1s^1 2s^1 2p^n$ configurations of neon.

Initial state	Final state	E_x	$100\omega\,(\alpha L_i S_i \rightarrow \alpha_f L_f S_i)$
$1s2s2p\ {}^2P_-$	$1s^22s\ {}^2S$	906.6	46.8
${}^2P_+$	${}^2S$	914.0	1.22
${}^4P$	${}^2S$	894.9	23.6[b]
$1s2s2p^2\ {}^1D$	$1s^22s2p\ {}^1P$	888.2	1.60
${}^3P_-$	${}^3P$	892.3	35.5
${}^3D$	${}^3P$	893.3	2.88
${}^1S$	${}^1P$	895.1	2.32
${}^1P$	${}^1P$	895.2	20.8
${}^3S$	${}^3P$	900.1	6.07
${}^3P_+$	${}^3P$	904.2	0.48
${}^5P$	${}^3P$	878.4	28.8[b]
$1s2s2p^3\ {}^2D_-$	$1s^22s2p^2\ {}^2P$	870.3	0.18
${}^2P_-$	${}^2P$	874.7	0.22
${}^2D_+$	${}^2P$	877.8	1.14
${}^2P_-$	${}^2S$	878.1	2.11
${}^4S_-$	${}^4P$	879.5	31.5
${}^2D_-$	${}^2D$	879.8	3.91
${}^4D$	${}^4P$	880.1	2.10
${}^2P_+$	${}^2P$	882.1	1.36
${}^2S$	${}^2P$	883.6	21.8
${}^2P_-$	${}^2D$	884.1	2.68
${}^4P$	${}^4P$	884.5	2.82
${}^2P_+$	${}^2S$	885.5	0.26
${}^2D_+$	${}^2D$	887.2	0.50
${}^2P_+$	${}^2D$	891.6	0.33
${}^4S_+$	${}^4P$	895.9	0.27
${}^6S$	${}^4P$	863.8	2.63[b]
$1s2s2p^4\ {}^3P_-$	$1s^22s2p^3\ {}^3S$	856.9	0.075
${}^1D$	${}^1P$	863.3	1.08
${}^3P_-$	${}^3P$	866.9	2.12
${}^1D$	${}^1D$	867.1	0.37
${}^3D$	${}^3P$	868.5	0.59
${}^3P_+$	${}^3S$	869.0	0.91
${}^1S$	${}^1P$	869.5	1.68
${}^1P$	${}^1P$	870.1	2.27
${}^3P_-$	${}^3D$	870.7	3.58
${}^5P$	${}^5S$	870.9	1.90
${}^3D$	${}^3D$	872.2	1.79
${}^1P$	${}^1D$	873.8	3.83
${}^3S$	${}^3P$	874.6	2.99
${}^3P_+$	${}^3P$	879.0	0.078
${}^3P_+$	${}^3D$	882.8	0.13
$1s2s2p^5\ {}^2P_-$	$1s^22s2p^4\ {}^2P$	852.8	0.26
${}^2P_-$	${}^2S$	856.4	0.61
${}^2P_+$	${}^2P$	860.2	1.06
${}^2P_-$	${}^2D$	861.7	3.09
${}^4P$	${}^4P$	862.6	2.03
${}^2P_+$	${}^2S$	863.8	0.052
${}^2P_+$	${}^2D$	869.1	0.27
$1s2s2p^6\ {}^1S$	$1s^22s2p^5\ {}^1P$	850.9	1.43
${}^3S$	${}^3P$	855.9	2.21

[a] These transition energies were calculated with the Hartree-Fock-Slater atomic model.

[b] All these transitions are not allowed by the electric dipole selection rules in the L-S coupling scheme. These calculations were performed in the intermediate coupling schemes.

TABLE V. Theoretical x-ray transition energies [a] E_x (in eV) and multiplet partial fluorescence yields $\omega(\alpha L_i S_i \rightarrow \alpha_f L_f S_i)$ for $1s^1 2p^n$ configurations of neon.

Initial state	Final state	E_x	$100\omega(\alpha L_i S_i \rightarrow \alpha_f L_f S_i)$
$1s2p^2\ {}^2D$	$1s^2 2p\ {}^2P$	904.0	3.15
${}^2P$	${}^2P$	905.7	100.
${}^2S$	${}^2P$	911.2	7.65[b]
${}^4P$	${}^2P$	895.9	7.13[b]
$1s2p^3\ {}^1P$	$1s^2 2p^2\ {}^1S$	889.6	3.74
${}^3D$	${}^3P$	889.6	2.19
${}^1D$	${}^1D$	891.4	6.35
${}^3S$	${}^3P$	891.8	100.
${}^3P$	${}^3P$	894.2	3.02
${}^1P$	${}^1D$	895.9	4.78
${}^5S$	${}^3P$	879.8	2.84[b]
$1s2p^4\ {}^2D$	$1s^2 2p^3\ {}^2P$	876.5	0.615
${}^2P$	${}^2P$	877.7	2.74
${}^4P$	${}^4S$	879.4	1.94
${}^2D$	${}^2D$	880.5	1.87
${}^2P$	${}^2D$	881.7	4.63
${}^2S$	${}^2P$	882.9	3.18
$1s2p^5\ {}^1P$	$1s^2 2p^4\ {}^1S$	865.5	0.664
${}^3P$	${}^3P$	869.8	2.06
${}^1P$	${}^1D$	871.1	3.38
$1s2p^6\ {}^2S$	$1s^2 2p^5\ {}^2P$	861.7	2.21

[a] These transition energies were calculated with the Hartree-Fock-Slater model.

[b] These transitions are not allowed by the electric dipole selection rules in the L-S coupling scheme. These calculations were performed in the intermediate coupling scheme. The multiplet partial fluorescence yields for the $1s2p^2\ {}^2S$ and the $1s2p^2\ {}^4P$ states are respectively 0.224 and 0.213 when the effects due to the configuration mixing are included.

which cannot decay radiatively or nonradiatively in the first order and in the L-S coupling scheme. However, this state can decay in the intermediate coupling scheme. The value of the total angular momentum can be only $\frac{5}{2}$ for ${}^6S$. There is mixing of this state with other states with $J=\frac{5}{2}$, namely ${}^4D$, ${}^2D_+$, ${}^2D_-$ and ${}^4P$ of the same electronic configuration $1s2s2p^3$. Using the techniques outlined by Condon and Shortley,[9] the mixing coefficients were obtained and the rates were calculated.

IV. DISCUSSION AND CONCLUSIONS

Using the theoretical techniques developed by Fano,[6] we have derived the expressions for the Auger rates of various spectroscopic terms of electronic configurations $1s^1 2s^2 2p^n$, $1s^1 2s^0 2p^n$, and $1s^1 2s^1 2p^n$ $(n=6\rightarrow 1)$. Explicit formulas for these cases have been presented.

The energies of the multiplets with the corresponding fluorescence yields are given for variously ionized neon. The values of the multiplet partial fluorescence yield depend sensitively on the multiplicity and the orbital angular momentum value of a term for a specific configuration.

It should be noted that most of the multiplets corresponding to a configuration overlap with the transitions for other configurations with the same number of electrons in the L-shell. The high-resolution spectral measurements for neon, reported so far in the literature, do not have sufficient resolution to distinguish between the various multiplets. Consequently, assumptions regarding the relative population of the terms would have to be made to analyze the data. As we have noted before,[5] the assumption of a statistical population is found to be invalid for the ${}^3P$ and ${}^1P$ terms doubly ionized neon $(1s^1 2s^2 2p^5)$, which are produced in the collision of different projectiles with neon. We believe that a careful experimental determination of the relative population of variously ionized neon would be most fruitful.

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