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THEORETICAL TRANSITION ENERGIES, LIFETIMES
AND FLUORESCENCE YIELDS FOR MULTIPLY-IONIZED
FLUORINE AND SILICON

by

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CHAPTER I

INTRODUCTION

Multiply-ionized atoms are produced in ion-atom collisions¹, and both laboratory-produced²⁻³ and naturally-occurring plasmas⁴⁻⁵. Some of the theoretical quantities needed in the analyses of the experimental data are transition rates for different modes of deexcitation, transition energies, and lifetimes.

There are mainly two different processes of deexcitation for an atom with one or more inner-shell vacancies. In the radiative case, an inner-shell vacancy is filled by an electron from a higher-lying shell and a photon is emitted. The competitive process is the ejection of an Auger electron instead of a photon, and for this reason it is called the non-radiative decay.

Bambynek et al.⁶ have an extensive review of the theoretical calculations and the experimental data for atoms with a single inner-shell vacancy. However, there are relatively few calculations for multiply-ionized atoms. Bhalla⁷ reported the differences in the fluorescence yields for $1s2s^2 2p^5$ (¹P) and (³P) states of neon. Later, the theoretical expressions for the Auger rates, the numerical values of the x-ray transition energies, and the multiplet partial fluorescence yields for various degrees of L-shell ionization for single⁸, and for double⁹⁻¹⁰ K-shell vacancy cases have been presented. Theoretical work for neon was performed also by Chen et al.¹¹. Recently, numerical results for argon¹² with double vacancy in the 2p-subshell, and total rates and line fluorescence yields for three-electron ions¹³ ($1s2s^2$, $1s2s2p$, $1s2p^2$) for $Z = 7, 8, 10, 16, 26$ have been reported. Tunnell et al.¹⁴ presented results

for $1s2s^m 2p^n$ ($m = 0-2$; $n = 0-6$) configurations of fluorine.

Consider an electronic configuration with an arbitrary number of open shells. One of the initial-state levels can be designated by quantum numbers $\alpha_i J_i$. Similarly, the resulting final-state after the x-ray transition will be represented by $\alpha_f J_f$. The number of atoms which 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 expressed 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 $t = 0$, $N(\alpha_i J_i)$:

$$\begin{aligned} N_x(\alpha_i J_i \rightarrow \alpha_f J_f) &= \int_0^{\infty} dt N(\alpha_i J_i) \Gamma_x(\alpha_i J_i \rightarrow \alpha_f J_f) \exp[-\Gamma(\alpha_i J_i)t] \\ &= N(\alpha_i J_i) \Gamma_x(\alpha_i J_i \rightarrow \alpha_f J_f) / \Gamma(\alpha_i J_i) . \end{aligned} \quad (1)$$

The line fluorescence yield is defined as the fraction of atoms which decay by $(\alpha_i J_i \rightarrow \alpha_f J_f)$ x-ray transition and can be written in terms of the appropriate x-ray rate and the total rate as

$$\omega(\alpha_i J_i \rightarrow \alpha_f J_f) = \frac{\Gamma_x(\alpha_i J_i \rightarrow \alpha_f J_f)}{\Gamma(\alpha_i J_i)} . \quad (2)$$

When both x-ray and Auger transitions are allowed, the multiplet partial fluorescence yield for a transition between two multiplets is given as

$$\omega(\alpha_i L_i S_i \rightarrow \alpha_f L_f S_f) = \frac{\Gamma_x(\alpha_i L_i S_i \rightarrow \alpha_f L_f S_f)}{\Gamma(\alpha_i L_i S_i)} . \quad (3)$$

If it is assumed that the initial levels are populated statistically, an average fluorescence yield for an electronic configuration can be defined as

$$\bar{\omega} = \frac{\sum_i (2L_i + 1)(2S_i + 1) \omega(\alpha_i L_i S_i)}{\sum_i (2L_i + 1)(2S_i + 1)} . \quad (4)$$

Several experimental studies¹⁵⁻¹⁷ have involved fluorine and silicon ions. Since detailed theoretical results have not been available for various configurations of fluorine and silicon, it is the purpose of this thesis to present a) Auger rates for different terms of various configurations of fluorine with single K-shell vacancy, b) x-ray transition energies, lifetimes and multiplet partial fluorescence yields for multiply-ionized fluorine with two K-shell vacancies and neon-like silicon with single K-shell vacancy, c) the numerical values of the multiplet factor which have not been previously available.

Chapter II contains a brief description of the atomic model used in this work, and the numerical values of the multiplet factor for a large number of cases.

CHAPTER II

THEORETICAL DEVELOPMENT

In this section the theoretical procedures to calculate the properties of ions are presented. A brief description of the Hartree-Fock-Slater atomic model is followed by the development of expressions for the transition rates. Atomic units ($e = m = \hbar = 1$) are used throughout this section unless stated otherwise.

A. Multiconfiguration Hartree-Fock-Slater Atomic Model

The total energy of an atomic system can be determined by the exact solution of the nonrelativistic Schrödinger equation

$$H\psi = E\psi \quad (5)$$

where ψ is the total antisymmetrized wave function, E is the total energy and H is the Hamiltonian. The Hamiltonian for an N -electron atomic system without the spin-orbit interaction is given as

$$H = \sum_{i=1}^N \left[-\frac{\nabla_i^2}{2} - \frac{Z}{r_i} \right] + \sum_{i,j} \frac{1}{r_{ij}} \quad (6)$$

The terms in the square brackets describe the motion of a single electron in the Coulomb field of the nucleus, and the second term is the electrostatic interaction between all pairs of electrons.

The exact solution of the Schrödinger's equation is possible only for single-electron systems. In the theory of atomic spectra for the many-electron system, the most useful approximation is the self-consistent Hartree-Fock (HF)¹⁸⁻¹⁹ method. In this method the total wave function for the N -electron system is approximated as an antisymmetric product of one-electron functions of the central-field type. The solution of the

HF equations which result from the minimization of the total energy for a single electronic configuration gives the radial part of the single-electron wave functions. The total energy of the system is expressed as

$$E = \sum_i q_i I(i) + \sum_{i,j} \sum_k a_{ijk} F^k(i,j) - \sum_{i,j} \sum_k b_{ijk} G^k(i,j) \quad (7)$$

where $I(i)$ denotes a one-electron integral term arising from the kinetic energy of the electron in the subshell i and its electrostatic interaction with the nucleus. $F^k(i,j)$ and $G^k(i,j)$ denote, respectively, Coulomb and exchange integrals between the pairs of electrons in the subshells i and j . These integrals are evaluated over the self-consistent radial functions and the allowed values of k depend on the subshells involved. Finally, q_i , a_{ijk} and b_{ijk} are the appropriate coefficients.

The presence of exchange terms in HF equations makes the calculations rather complex and time-consuming. One simplification is to replace these exchange terms by an average potential which was proposed by Slater²⁰. The general form of this potential is given as

$$V_{\text{exch}}(r) = -3\alpha \left[\frac{3}{8\pi} \rho(r) \right]^{1/3} \quad (8)$$

where $\alpha = 1$ indicates Slater exchange while $\alpha = 2/3$ signifies Kohn and Sham²¹, and Gaspar²² (KSG) exchange. An inhomogeneity correction has been added to KSG exchange by Herman, Van Dyke, and Ortenburger²³ (HVO). In this work HVO exchange approximation

$$V_{\text{exch}}(r) = \left\{ \alpha + \beta \frac{1}{\rho^{2/3}} \left[\frac{4}{3} \left(\frac{\nabla \rho}{\rho} \right)^2 - 2 \frac{\nabla^2 \rho}{\rho} \right] \right\} \left\{ -3 \left[\frac{3}{8\pi} \rho(r) \right]^{1/3} \right\} \quad (9)$$

is used with $\beta = 0.0028$. Finally, a "Latter tail"²⁴ correction is added to the potential.

Hartree-Fock-Slater bound state wave functions were obtained by solving the following equation numerically:

$$\left[-\frac{1}{2} \frac{d^2}{dr^2} + \frac{l(l+1)}{2r^2} + v(r) \right] P_{nl}(r) = E_{nl} P_{nl}(r) \quad (10)$$

where the central potential is given by

$$V(r) = -\frac{Z}{r} + \int \frac{\rho(r')}{|r-r'|} d^3r' + V_{\text{exch}}(r) \quad (11)$$

The computer program of Herman and Skilman²⁵ was modified for the exchange approximation and used to obtain bound state solutions. The continuum wave functions needed for the calculations of Auger rates were calculated using the central potential developed for bound state solutions.

A better approximation to obtain the wave functions is to write the wave function as a linear combination of Slater determinants for single configurations:

$$\psi(\alpha LS) = \sum_i c_i \psi(\alpha_i LS) \quad (12)$$

This procedure is called Multiconfiguration Hartree-Fock-Slater (MCHFS) method and has been used in some of the calculations presented here.

B. X-Ray Transition Rates

The transition rates are calculated from first order perturbation theory according to Fermi's Golden Rule

$$\Gamma(i \rightarrow f) = 2\pi \rho_f |\langle f | H' | i \rangle|^2 \quad (13)$$

where i and f denote the initial state and the final state, respectively.

The density of the final states is designated by ρ_f , and the matrix element is calculated for the perturbation H' .

Without the inclusion of the configuration mixing, x-ray transition rate between the atomic levels in the nonrelativistic electric dipole approximation is given²⁶ as

$$\Gamma_x(\alpha_i L_i S_i J_i \rightarrow \alpha_f L_f S_f J_f) = \frac{4}{3} k^3 (2J_i + 1)^{-1} \times [R_{line}(S_i L_f J_f, S_i L_i J_i) R_{mult}(\alpha_f L_f, \alpha_i L_i) \times (-1)^{l-l'} \sqrt{l} I(nl, n'l')]^2. \quad (14)$$

In a similar way, the x-ray rate for a transition between the multiplets can be written²⁶ as

$$\Gamma_x(\alpha_i L_i S_i \rightarrow \alpha_f L_f S_f) = \frac{4}{3} k^3 (2L_i + 1)^{-1} \times [R_{mult}(\alpha_f L_f, \alpha_i L_i) (-1)^{l-l'} \sqrt{l} I(nl, n'l')]^2. \quad (15)$$

In Equations (14-15) the wave vector k is the ratio of the transition energy to the speed of light ($c = 137$ in atomic units), and the transition integral is defined as

$$I(nl, n'l') = \int_0^\infty P_{nl}(r) P_{n'l'}(r) r dr. \quad (16)$$

The multiplet factor, R_{mult} , depends upon the two particular configurations involved in the transition and can be expressed in terms of Racah coefficients. The numerical values of the multiplet factor for a large number of cases have been tabulated and can be found in the literature²⁶. However, for many cases the multiplet factor need to be calculated. One of the major efforts in this thesis was the evaluation of the multiplet factor. Tables Ia, Ib, Ic, Id, and Ie contain the numerical values of the multiplet factor for various x-ray transitions.

C. Auger Transition Rates

The Auger process is the result of Coulomb repulsion between two electrons. The transition rate in the perturbation theory is given as

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TABLE Ia: Multiplet factors, $R_{\text{mult}} (\alpha_f L_f, \alpha_i L_i)$, for $1s2p^n 3s (\alpha_i L_i S_i) \rightarrow 1s2p^{n+1} (\alpha_f L_f S_f)$ transitions.

Initial state*		Final state	R_{mult}
1 s	3 s	1 s 2 p	
	1S	1P	1
	3S	3P	1
1 s 2 p 3 s		1 s 2 p ²	
(1P)	2P]	2S	$-1/\sqrt{6}$
	2P]	2P	$\sqrt{3/2}$
	2P]	2D	$-\sqrt{5/6}$
(3P)	2P]	2S	$1/\sqrt{2}$
	2P]	2P	$1/\sqrt{2}$
	2P]	2D	$\sqrt{5/2}$
"	4P	4P	$\sqrt{2}$
1 s 2 p ² 3 s		1 s 2 p ³	
	1S	1P	$\sqrt{2/3}$
	3S	3P	$\sqrt{2/3}$
	1P]	1P	$-\sqrt{3/2}$
	1P]	1D	$\sqrt{5/2}$
(2P)	3P]	3S	$\sqrt{8/9}$
	3P]	3P	$1/\sqrt{6}$
	3P]	3D	$-\sqrt{5/18}$
(4P)	3P]	3S	$1/3$
	3P]	3P	$-\sqrt{4/3}$
	3P]	3D	$\sqrt{20/9}$
"	5P	5S	1
	1D]	1P	$-\sqrt{5/6}$
	1D]	1D	$-\sqrt{5/2}$
	3D]	3P	$-\sqrt{5/6}$
	3D]	3D	$-\sqrt{5/2}$
1 s 2 p ³ 3 s		1 s 2 p ⁴	
	2S	2P	$-\sqrt{4/3}$
(3S)	4S	4P	$1/\sqrt{12}$

Initial state		Final state	R_{mult}
(⁵ S)	⁴ S	⁴ P	$\sqrt{5/4}$
(¹ P)	² P	² S	$-1/\sqrt{3}$
	² P	² P	$-\sqrt{3/4}$
	² P	² D	$\sqrt{5/12}$
(³ P)	² P	² S	1
	² P	² P	$-1/2$
	² P	² D	$-\sqrt{5/4}$
"	⁴ P	⁴ P	-1
(¹ D)	² D	² P	$\sqrt{5/4}$
	² D	² D	$\sqrt{5/4}$
(³ D)	² D	² P	$\sqrt{5/12}$
	² D	² D	$-\sqrt{15/4}$
"	⁴ D	⁴ P	$\sqrt{5/3}$
$1s2p^43s$		$1s2p^5$	
	¹ S	¹ P	$1/\sqrt{3}$
	³ S	³ P	$1/\sqrt{3}$
	¹ P	¹ P	$\sqrt{3}$
(² P)	³ P	³ P	$-1/\sqrt{3}$
(⁴ P)	³ P	³ P	$\sqrt{8/3}$
	¹ D	¹ P	$\sqrt{5/3}$
	³ D	³ P	$\sqrt{5/3}$
$1s2p^53s$		$1s2p^6$	
(¹ P)	² P	² S	$-1/\sqrt{2}$
(³ P)	² P	² S	$\sqrt{3/2}$

* The notation used in some of the tables (Tables Ia through Ie, and Table IVb) is as follows: $1s2p(^1P)3s$ is written as $1s2p3s$.
 (^1P)

TABLE Ib: Multiplet factors, $R_{\text{mult}}(\alpha_f L_f, \alpha_i L_i)$, for $1s2p^n 3s^2 (\alpha_i L_i S_i) \rightarrow 1s2p^{n+1} 3s (\alpha_f L_f S_f)$ transitions.

Initial state	Final state	R_{mult}
$1s \quad 3s^2$	$1s 2p 3s$	
$\left. \begin{array}{c} {}^2S \\ {}^2S \end{array} \right\}$	$\begin{array}{c} ({}^1P) \quad {}^2P \\ ({}^3P) \quad {}^2P \end{array}$	$\begin{array}{c} -1/\sqrt{2} \\ \sqrt{3/2} \end{array}$
$1s 2p 3s^2$	$1s 2p^2 3s$	
$\left. \begin{array}{c} {}^1P \\ {}^1P \\ {}^1P \end{array} \right\}$	$\begin{array}{c} {}^1S \\ {}^1P \\ {}^1D \end{array}$	$\begin{array}{c} -1/\sqrt{3} \\ \sqrt{3} \\ -\sqrt{5/3} \end{array}$
$\left. \begin{array}{c} {}^3P \\ {}^3P \\ {}^3P \\ {}^3P \end{array} \right\}$	$\begin{array}{c} ({}^2P) \quad {}^3S \\ ({}^4P) \quad {}^3P \\ {}^3P \\ {}^3D \end{array}$	$\begin{array}{c} -1/\sqrt{3} \\ -1/\sqrt{3} \\ \sqrt{8/3} \\ -\sqrt{5/3} \end{array}$
$1s 2p^2 3s^2$	$1s 2p^3 3s$	
$\left. \begin{array}{c} {}^2S \\ {}^2S \end{array} \right\}$	$\begin{array}{c} ({}^1P) \quad {}^2P \\ ({}^3P) \quad {}^2P \end{array}$	$\begin{array}{c} -1/\sqrt{3} \\ 1 \end{array}$
$\left. \begin{array}{c} {}^2P \\ {}^2P \\ {}^2P \\ {}^2P \\ {}^2P \end{array} \right\}$	$\begin{array}{c} ({}^1P) \quad {}^2S \\ ({}^3P) \quad {}^2P \\ ({}^1D) \quad {}^2P \\ ({}^3D) \quad {}^2D \end{array}$	$\begin{array}{c} \sqrt{4/3} \\ \sqrt{3/4} \\ 1/2 \\ -\sqrt{5/4} \end{array}$
$\left. \begin{array}{c} {}^4P \\ {}^4P \\ {}^4P \\ {}^4P \end{array} \right\}$	$\begin{array}{c} ({}^3S) \quad {}^2D \\ ({}^5S) \quad {}^2D \end{array}$	$\begin{array}{c} -\sqrt{5/12} \\ -1/\sqrt{12} \end{array}$
$\left. \begin{array}{c} {}^4P \\ {}^4P \end{array} \right\}$	$\begin{array}{c} {}^4S \\ {}^4S \end{array}$	$\begin{array}{c} \sqrt{5/4} \\ 1 \end{array}$
$\left. \begin{array}{c} {}^2D \\ {}^2D \\ {}^2D \\ {}^2D \end{array} \right\}$	$\begin{array}{c} {}^4P \\ {}^4D \\ ({}^1P) \quad {}^2P \\ ({}^3P) \quad {}^2P \end{array}$	$\begin{array}{c} -\sqrt{5/3} \\ \sqrt{5/12} \\ -\sqrt{5/4} \end{array}$
$\left. \begin{array}{c} {}^2D \\ {}^2D \end{array} \right\}$	$\begin{array}{c} ({}^1D) \quad {}^2D \\ ({}^3D) \quad {}^2D \end{array}$	$\begin{array}{c} \sqrt{5/4} \\ -\sqrt{15/4} \end{array}$
$1s 2p^3 3s^2$	$1s 2p^4 3s$	
$\left. \begin{array}{c} {}^3S \\ {}^3S \end{array} \right\}$	$\begin{array}{c} ({}^2P) \quad {}^3P \\ ({}^4P) \quad {}^3P \end{array}$	$\begin{array}{c} \sqrt{8/9} \\ 1/3 \end{array}$

Initial state	Final state	R_{mult}
5S	"	5P
1P		1S
1P		1P
1P		1D
3P		3S
3P	(^2P)	3P
3P	(^4P)	3P
3P		3D
1D		1P
1D		1D
3D	(^2P)	3P
3D	(^4P)	3P
3D		3D
$1s2p^43s^2$	$1s2p^53s$	
2S	(^1P)	2P
2S	(^3P)	2P
2P	(^1P)	2P
2P	(^3P)	2P
4P	"	4P
2D	(^1P)	2P
2D	(^3P)	2P
$1s2p^53s^2$	$1s2p^63s$	
1P		1S
3P		3S

TABLE Ic: Multiplet factors, $R_{\text{mult}}(\alpha_f L_f, \alpha_i L_i)$, for $1s2p^n 3s2s$
 $(\alpha_i L_i S_i) \rightarrow 1s2p^{n+1} 2s (\alpha_f L_f S_f)$ transitions.

Initial state			final state		R_{mult}
1 s	3 s 2 s		1 s 2 p	2 s	
	(¹ s)	² S	(¹ p)	² P	1
	(³ s)	² S	(³ p)	² P	1
	"	⁴ S	"	⁴ P	1
1 s 2 p	3 s 2 s		1 s 2 p ²	2 s	
	(¹ p) (² p)	¹ P		¹ S	$-\frac{1}{\sqrt{6}}$
		¹ P		¹ P	$\frac{\sqrt{3}}{2}$
		¹ P		¹ D	$-\frac{\sqrt{5}}{6}$
	(³ p) (² p)	¹ P		¹ S	$\frac{1}{\sqrt{2}}$
		¹ P		¹ P	$\frac{1}{\sqrt{2}}$
		¹ P		¹ D	$\frac{\sqrt{5}}{2}$
	(¹ p) (² p)	³ P	(² s)	³ S	$-\frac{1}{\sqrt{6}}$
		³ P	(² p)	³ P	$\frac{\sqrt{3}}{2}$
		³ P	(² D)	³ D	$-\frac{\sqrt{5}}{6}$
	(³ p) (² p)	³ P	(² s)	³ S	$\frac{1}{\sqrt{2}}$
		³ P	(² p)	³ P	$\frac{1}{\sqrt{2}}$
		³ P	(² D)	³ D	$\frac{\sqrt{5}}{2}$
	(³ p) (⁴ p)	³ P	(⁴ p)	³ P	$\sqrt{2}$
	"	⁵ P	"	⁵ P	$\sqrt{2}$
1 s 2 p ²	3 s 2 s		1 s 2 p ³	2 s	
	(¹ s)	² S	(¹ p)	² P	$\frac{\sqrt{2}}{3}$
	(³ s)	² S	(³ p)	² P	$\frac{\sqrt{2}}{3}$
	"	⁴ S	"	⁴ P	$\frac{\sqrt{2}}{3}$
	(² p) (¹ p)	² P	(¹ p)	² P	$-\frac{\sqrt{3}}{2}$
		² P	(¹ D)	² D	$\frac{\sqrt{5}}{2}$
	(² p) (³ p)	² P	(³ s)	² S	$\frac{\sqrt{8}}{9}$
		² P	(³ p)	² P	$\frac{1}{\sqrt{6}}$
		² P	(³ D)	² D	$-\frac{\sqrt{5}}{18}$
	(⁴ p) (³ p)	² P	(³ s)	² S	$\frac{1}{3}$
		² P	(³ p)	² P	$-\frac{\sqrt{4}}{3}$
		² P	(³ D)	² D	$\frac{\sqrt{20}}{9}$

TABLE Ic: continued

Initial state		Final state		R _{mult}
(² P) (³ P)	⁴ P	(³ S)	⁴ S	$\sqrt{8/9}$
	⁴ P		⁴ P	$1/\sqrt{6}$
	⁴ P		⁴ D	$-\sqrt{5/18}$
(⁴ P) (³ P)	⁴ P	(³ S)	⁴ S	$1/3$
	⁴ P		⁴ P	$-\sqrt{4/3}$
	⁴ P		⁴ D	$\sqrt{20/9}$
(⁴ P) (⁵ P)	⁴ P	(⁵ S)	⁴ S	1
"	⁶ P	"	⁶ S	1
(¹ D)	² D	(¹ P)	² P	$-\sqrt{5/6}$
	² D	(¹ D)	² D	$-\sqrt{5/2}$
(³ D)	² D	(³ P)	² P	$-\sqrt{5/6}$
	² D	(³ D)	² D	$-\sqrt{5/2}$
"	⁴ D		⁴ P	$-\sqrt{5/6}$
"	⁴ D		⁴ D	$-\sqrt{5/2}$
1 s 2 p ³ 3 s 2 s		1 s 2 p ⁴ 2 s		
	¹ S		¹ P	$-\sqrt{4/3}$
(³ S) (² S)	³ S	(² P)	³ P	$-\sqrt{4/3}$
(³ S) (⁴ S)	³ S	(⁴ P)	³ P	$1/\sqrt{12}$
(⁵ S) (⁴ S)	³ S	(⁴ P)	³ P	$-\sqrt{5/4}$
(³ S) (⁴ S)	⁵ S	"	⁵ P	$1/\sqrt{12}$
(⁵ S) (⁴ S)	⁵ S	"	⁵ P	$-\sqrt{5/4}$
(¹ P) (² P)	¹ P		¹ S	$-1/\sqrt{3}$
	¹ P		¹ P	$-\sqrt{3/4}$
	¹ P		¹ D	$\sqrt{5/12}$
(³ P) (² P)	¹ P		¹ S	1
	¹ P		¹ P	$-1/2$
	¹ P		¹ D	$-\sqrt{5/4}$
(¹ P) (² P)	³ P		³ S	$-1/\sqrt{3}$
	³ P	(² P)	³ P	$-\sqrt{3/4}$
	³ P		³ D	$\sqrt{5/12}$
(³ P) (² P)	³ P		³ S	1
	³ P	(² P)	³ P	$-1/2$
	³ P		³ D	$-\sqrt{5/4}$
(³ P) (⁴ P)	³ P	(⁴ P)	³ P	-1
"	⁵ P	"	⁵ P	-1

Initial state		Final state		R _{mult}
(¹ D) (² D)	¹ D]		¹ P	$\sqrt{5/4}$
	¹ D]		¹ D	$\sqrt{5/4}$
(³ D) (² D)	¹ D]		¹ P	$\sqrt{5/12}$
	¹ D]		¹ D	$-\sqrt{15/4}$
(¹ D) (² D)	³ D]	(² P)	³ P	$\sqrt{5/4}$
	³ D]		³ D	$\sqrt{5/4}$
(³ D) (² D)	³ D]	(² P)	³ P	$\sqrt{5/12}$
	³ D]		³ D	$-\sqrt{15/4}$
(³ D) (⁴ D)	³ D	(⁴ P)	³ P	$\sqrt{5/3}$
"	⁵ D	"	⁵ P	$\sqrt{5/3}$
1 s 2 p ⁴ 3 s 2 s		1 s 2 p ⁵ 2 s		
(¹ S)	² S	(¹ P)	² P	$1/\sqrt{3}$
(³ S)	² S	(³ P)	² P	$1/\sqrt{3}$
"	⁴ S	"	⁴ P	$1/\sqrt{3}$
(² P) (¹ P)	² P	(¹ P)	² P	$\sqrt{3}$
(² P) (³ P)	² P	(³ P)	² P	$-1/\sqrt{3}$
(⁴ P) (³ P)	² P	(³ P)	² P	$\sqrt{8/3}$
(² P) (³ P)	⁴ P	"	⁴ P	$-1/\sqrt{3}$
(⁴ P) (³ P)	⁴ P	"	⁴ P	$\sqrt{8/3}$
(¹ D)	² D	(¹ P)	² P	$\sqrt{5/3}$
(³ D)	² D	(³ P)	² P	$\sqrt{5/3}$
"	⁴ D	"	⁴ P	$\sqrt{5/3}$
1 s 2 p ⁵ 3 s 2 s		1 s 2 p ⁶ 2 s		
(¹ P) (² P)	¹ P		¹ S	$-1/\sqrt{2}$
(³ P) (² P)	¹ P		¹ S	$\sqrt{3/2}$
(¹ P) (² P)	³ P		³ S	$-1/\sqrt{2}$
(³ P) (² P)	³ P		³ S	$\sqrt{3/2}$

TABLE Id: Multiplet factor, $R_{\text{mult}}(\alpha_f L_f, \alpha_i L_i)$, for $1s2p^n 3s^2 2s (\alpha_i L_i S_i) \rightarrow 1s2p^{n+1} 3s2s (\alpha_f L_f S_f)$ transitions.

Initial state	Final state	R_{mult}
$1s \quad 3s^2 2s$	$1s 2p 3s 2s$	
1S	$(^1P) (^2P) \quad ^1P$	$-1/\sqrt{2}$
1S	$(^3P) \quad " \quad ^1P$	$\sqrt{3/2}$
3S	$(^1P) \quad " \quad ^3P$	$-1/\sqrt{2}$
3S	$(^3P) \quad " \quad ^3P$	$\sqrt{3/2}$
$1s 2p 3s^2 2s$	$1s 2p^2 3s 2s$	
(^1P)	$(^1S) \quad ^2S$	$-1/\sqrt{3}$
2P	$(^1P) \quad ^2P$	$\sqrt{3}$
2P	$(^1D) \quad ^2D$	$-\sqrt{5/3}$
(^3P)	$(^3S) \quad ^2S$	$-1/\sqrt{3}$
2P	$(^2P) \quad ^2P$	$-1/\sqrt{3}$
2P	$(^4P) \quad ^2P$	$\sqrt{8/3}$
2P	$(^3D) \quad ^2D$	$-\sqrt{5/3}$
$"$	4S	$-1/\sqrt{3}$
$"$	$(^2P) \quad ^4P$	$-1/\sqrt{3}$
$"$	$(^4P) (^3P) \quad ^4P$	$\sqrt{8/3}$
$"$	4D	$-\sqrt{5/3}$
$1s 2p^2 3s^2 2s$	$1s 2p^3 3s 2s$	
1S	$(^1P) \quad ^1P$	$-1/\sqrt{3}$
1S	$(^3P) \quad ^1P$	1
3S	$(^1P) \quad ^3P$	$-1/\sqrt{3}$
3S	$(^3P) (^2P) \quad ^3P$	1
1P	1S	$\sqrt{4/3}$
1P	$(^1P) \quad ^1P$	$\sqrt{3/4}$
1P	$(^3P) \quad ^1P$	$1/2$
1P	$(^1D) \quad ^1D$	$-\sqrt{5/4}$
1P	$(^3D) \quad ^1D$	$-\sqrt{5/12}$
(^2P)	$(^2S) \quad ^3S$	$\sqrt{4/3}$
3P	$(^1P) \quad ^3P$	$\sqrt{3/4}$
3P	$(^3P) (^2P) \quad ^3P$	$1/2$
3P	$(^1D) \quad ^3D$	$-\sqrt{5/4}$

Initial state		Final state		R _{mult}
(4p)	3P	$(^3D) (^2D)$	3D	$-\sqrt{5/12}$
	3P	$(^3S) (^4S)$	3S	$-1/\sqrt{12}$
	3P	$(^5S) "$	3S	$\sqrt{5/4}$
	3P	(^4P)	3P	1
	3P	(^4D)	3D	$-\sqrt{5/3}$
	5P	(^3S)	5S	$-1/\sqrt{12}$
	5P	$(^5S) (^4S)$	5S	$\sqrt{5/4}$
	5P		5P	1
	5P		5D	$-\sqrt{5/3}$
	1D	(^1P)	1P	$\sqrt{5/12}$
"	1D	(^3P)	1P	$-\sqrt{5/4}$
	1D	(^1D)	1D	$\sqrt{5/4}$
	1D	(^3D)	1D	$-\sqrt{15/4}$
	3D	(^1P)	3P	$\sqrt{5/12}$
	3D	$(^3P) (^2P)$	3P	$-\sqrt{5/4}$
	3D	(^1D)	3D	$\sqrt{5/4}$
	3D	$(^3D) (^2D)$	3D	$-\sqrt{15/4}$
$1s2p^33s^22s$		$1s2p^43s2s$		
(3s)	2S	$(^2P) (^3P)$	2P	$\sqrt{8/9}$
	2S	$(^4P) "$	2P	1/3
	4S	$(^2P) "$	4P	$\sqrt{8/9}$
	4S	$(^4P) (^3P)$	4P	1/3
(5s)	4S	(^5P)	4P	1
"	6S	"	6P	1
(1p)	2P	(^1S)	2S	$-\sqrt{2/3}$
(3p)	2P	$(^2P) (^1P)$	2P	$-\sqrt{3/2}$
	2P	$(^2D) (^1D)$	2D	$\sqrt{5/6}$
	2P	(^3S)	2S	$-\sqrt{2/3}$
	2P	$(^2P) (^3P)$	2P	$1/\sqrt{6}$
	2P	$(^4P) "$	2P	$-\sqrt{4/3}$
	2P	(^3D)	2D	$\sqrt{5/6}$
	4P		4S	$-\sqrt{2/3}$
	4P	(^2P)	4P	$1/\sqrt{6}$
"	4P	$(^4P) (^3P)$	4P	$-\sqrt{4/3}$
"	4P		4D	$\sqrt{5/6}$

Initial state		Final state		R_{mult}
(^1D)	2D	$(^2P) (^1P)$	2P	$\sqrt{5/2}$
	2D	$(^2D) (^1D)$	2D	$\sqrt{5/2}$
(^3D)	2D	$(^2P) (^3P)$	2P	$-\sqrt{5/18}$
	2D	$(^4P) "$	2P	$\sqrt{20/9}$
	2D	(^3D)	2D	$\sqrt{5/2}$
"	4D	(^2P)	4P	$-\sqrt{5/18}$
"	4D	$(^4P) (^3P)$	4P	$\sqrt{20/9}$
"	4D		4D	$\sqrt{5/2}$
$1s 2p^4 3s^2 2s$		$1s 2p^5 3s 2s$		
	1S	(^1P)	1P	$-1/\sqrt{6}$
	1S	(^3P)	1P	$1/\sqrt{2}$
	3S	(^1P)	3P	$-1/\sqrt{6}$
	3S	$(^3P) (^2P)$	3P	$1/\sqrt{2}$
	1P	$(^1P) "$	1P	$-\sqrt{3/2}$
	1P	$(^3P) "$	1P	$-1/\sqrt{2}$
(^2P)	3P	$(^1P) "$	3P	$-\sqrt{3/2}$
	3P	$(^3P) (^2P)$	3P	$-1/\sqrt{2}$
(^4P)	3P	$(^3P) (^4P)$	3P	$-\sqrt{2}$
"	5P	"	5P	$-\sqrt{2}$
	1D	(^1P)	1P	$-\sqrt{5/6}$
	1D	(^3P)	1P	$\sqrt{5/2}$
	3D	(^1P)	3P	$-\sqrt{5/6}$
	3D	$(^3P) (^2P)$	3P	$\sqrt{5/2}$
$1s 2p^5 3s^2 2s$		$1s 2p^6 3s 2s$		
(^1P)	2P	(^1S)	2S	-1
(^3P)	2P	(^3S)	2S	-1
"	4P	"	4S	-1

TABLE Ie: Multiplet factor, $R_{\text{mult}}(\alpha_f L_f, \alpha_i L_i)$, for $1s2p^{n-1}3s2s (\alpha_i L_i S_i) \rightarrow 1s^2 2p^n 3s2s (\alpha_f L_f S_f)$ transitions.

Initial state	Final state	R_{mult}
$1s2p3s2s$	$1s^2 3s2s$	
$(^1p)(^2p) \quad ^1P$	1S	$\sqrt{2}$
$(^1p)(^2p) \quad ^3P$	3S	$\sqrt{2}$
$1s2p^23s2s$	$1s^2 2p3s2s$	
$(^1s) \quad ^2S$	$(^1p) \quad ^2P$	$-1/\sqrt{3}$
$(^3s) \quad ^2S$	$(^3p) \quad ^2P$	$-1/\sqrt{3}$
" 4S	" 4P	$-1/\sqrt{3}$
$(^1p) \quad ^2P$	$(^1p) \quad ^2P$	$\sqrt{3}$
$(^2p)(^3p) \quad ^2P$	$(^3p) \quad ^2P$	$\sqrt{3}$
$(^2p)(^3p) \quad ^4P$	" 4P	$\sqrt{3}$
$(^1D) \quad ^2D$	$(^1p) \quad ^2P$	$-\sqrt{5/3}$
$(^3D) \quad ^2D$	$(^3p) \quad ^2P$	$-\sqrt{5/3}$
" 4D	" 4P	$-\sqrt{5/3}$
$1s2p^33s2s$	$1s^2 2p^2 3s2s$	
1S	1P	$\sqrt{4/3}$
$(^3s)(^2s) \quad ^3S$	$(^3p)(^2p) \quad ^3P$	$\sqrt{4/3}$
$(^3s)(^4s) \quad ^3S$	$(^3p)(^4p) \quad ^3P$	$\sqrt{4/3}$
$(^3s)(^4s) \quad ^5S$	" 5P	$\sqrt{4/3}$
$(^1p)(^2p) \quad ^1P$	1S	$\sqrt{4/3}$
1P	1D	$-\sqrt{5/3}$
$(^3p)(^2p) \quad ^1P$	1P	1
$(^1p)(^2p) \quad ^3P$	3S	$\sqrt{4/3}$
3P	3D	$-\sqrt{5/3}$
$(^3p)(^2p) \quad ^3P$	$(^2p) \quad ^3P$	1
$(^3p)(^4p) \quad ^3P$	$(^4p) \quad ^3P$	1
" 5P	" 5P	1
$(^1D)(^2D) \quad ^1D$	1D	$\sqrt{5}$
$(^3D)(^2D) \quad ^1D$	1P	$\sqrt{5/3}$
$(^1D)(^2D) \quad ^3D$	3D	$\sqrt{5}$
$(^3D)(^2D) \quad ^3D$	$(^2p) \quad ^3P$	$\sqrt{5/3}$
$(^3D)(^4D) \quad ^3D$	$(^4p) \quad ^3P$	$\sqrt{5/3}$

Initial state		Final state		R _{mult}
	" ⁵ D	" ⁵ P		$\sqrt{5/3}$
1 s 2 p ⁴ 3 s 2 s		1 s ² 2 p ³ 3 s 2 s		
(¹ S)	² S	(¹ P)	² P	$-\sqrt{2/3}$
(³ S)	² S	(³ P)	² P	$-\sqrt{2/3}$
"	⁴ S	"	⁴ P	$-\sqrt{2/3}$
(² P) (¹ P)	² P]	(¹ P)	² P	$-\sqrt{3/2}$
	² P]	(¹ D)	² D	$-\sqrt{5/2}$
(² P) (³ P)	² P]	(³ P)	² P	$-\sqrt{3/2}$
	² P]	(³ D)	² D	$-\sqrt{5/2}$
(⁴ P) (³ P)	² P	(³ S)	² S	1
(² P) (³ P)	⁴ P]		⁴ P	$-\sqrt{3/2}$
	⁴ P]		⁴ D	$-\sqrt{5/2}$
(⁴ P) (³ P)	⁴ P	(³ S)	⁴ S	1
(⁴ P) (⁵ P)	⁴ P	(⁵ S)	⁴ S	1
"	⁶ P	"	⁶ S	1
(² D) (¹ D)	² D]	(¹ P)	² P	$\sqrt{5/6}$
	² D]	(¹ D)	² D	$-\sqrt{5/2}$
(² D) (³ D)	² D]	(³ P)	² P	$\sqrt{5/6}$
	² D]	(³ D)	² D	$-\sqrt{5/2}$
"	⁴ D]		⁴ P	$\sqrt{5/6}$
"	⁴ D]		⁴ D	$-\sqrt{5/2}$
1 s 2 p ⁵ 3 s 2 s		1 s ² 2 p ⁴ 3 s 2 s		
(¹ P) (² P)	¹ P]		¹ S	$\sqrt{2/3}$
	¹ P]		¹ D	$\sqrt{10/3}$
(³ P) (² P)	¹ P		¹ P	$-\sqrt{2}$
(¹ P) (² P)	³ P]	(² S)	³ S	$\sqrt{2/3}$
	³ P]	(² D)	³ D	$\sqrt{10/3}$
(³ P) (² P)	³ P	(² P)	³ P	$-\sqrt{2}$
(⁴ P)	³ P	(⁴ P)	³ P	$-\sqrt{2}$
"	⁵ P	"	⁵ P	$-\sqrt{2}$
1 s 2 p ⁶ 3 s 2 s		1 s ² 2 p ⁵ 3 s 2 s		
(¹ S)	² S	(¹ P)	² P	1
(³ S)	² S	(³ P)	² P	1
"	⁴ S	"	⁴ P	-1

$$\Gamma_A(i \rightarrow f) = 2\pi \rho_f \left| \langle f | \sum_{ij} \frac{1}{r_{ij}} | i \rangle \right|^2 \quad (17)$$

where $|i\rangle$ and $|f\rangle$ are antisymmetrized wave functions.

Consider the case of a single initial vacancy ($n_3 \ell_3$) and all other shells be fully occupied. The Auger rate for the transition ($n_3 \ell_3 - n_1 \ell_1, n_2 \ell_2$), where the continuum electron is designated by $k \ell_4$, is given by

$$\begin{aligned} \Gamma_A(i \rightarrow f) = & \frac{2J+1}{2(2\ell_3+1)} 2\pi \left| \tau \sum_k \left[R^k(1,2,3,4) \langle \ell_3 \| C^k \| \ell_1 \rangle \langle \ell_k \| C^k \| \ell_2 \rangle \begin{Bmatrix} \ell_3 & \ell_4 & L \\ \ell_2 & \ell_1 & k \end{Bmatrix} \right. \right. \\ & \left. \left. + (-)^{L+S} R^k(1,2,3,4) \langle \ell_3 \| C^k \| \ell_2 \rangle \langle \ell_k \| C^k \| \ell_1 \rangle \begin{Bmatrix} \ell_3 & \ell_4 & L \\ \ell_1 & \ell_2 & k \end{Bmatrix} \right] \right|^2 \quad (18) \end{aligned}$$

where the reduced matrix elements are written in terms of 3-J symbols as

$$\langle \ell \| C^k \| \ell' \rangle = \sqrt{2\ell+1} \sqrt{2\ell'+1} \begin{pmatrix} \ell' & k & \ell \\ 0 & 0 & 0 \end{pmatrix} (-)^{\ell} \quad (19)$$

and the Slater integrals are given as

$$R^k(1,2,3,4) = \int_0^\infty \int_0^\infty P_{n_1 \ell_1}(i) P_{n_2 \ell_2}(j) \frac{r_{ij}^k}{(r_{ij})^{k+1}} P_{n_3 \ell_3}(i) P_{n_4 \ell_4}(j) dr_i dr_j \quad (20)$$

When there are more than one open shell in the initial state, as in the case of multiply-ionized atoms, special techniques²⁷ are required to calculate the matrix elements. The theoretical formulas for neon-like atoms with different number of electrons in the L-shell have been derived by Bhalla⁸.

The next chapter contains the theoretical results. A brief explanation of the decay of metastable states in the intermediate coupling is also given.

CHAPTER III

NUMERICAL RESULTS

In this chapter the numerical results of the calculations for multiply-ionized fluorine and silicon are presented. Tables IIa, IIb, and IIc contain theoretical x-ray transition energies, lifetimes, and multiplet partial fluorescence yields for $2s^m 2p^n$ configurations of fluorine. The same type of information for $1s 2s^m 2p^n$ configurations of silicon is presented in Tables IIIa, IIIb, and IIIc. The theoretical Auger rates for different terms of $1s 2s^m 2p^n$ configurations of fluorine are given in Tables IVa, IVb, and IVc. Theoretical average fluorescence yields for $1s 2s^m 2p^n$ configurations of various elements (N, O, F, Ne, and Si) are presented in Table V.

All calculations were performed in the LS-coupling scheme. The x-ray transition energies were calculated by computing the difference of the total energy of the atom in the initial and final states.

There are some additional remarks which need to be made concerning the calculations. For some configurations there is at least one pair of terms with the same values of S and L. One example is the two 4S terms of $1s 2s 2p^3$ configuration. The wave functions for these terms can be written as a linear combination of the two theoretical states with the same S and L values:

$$\Phi_1(^4S) = a_{11} \psi_1 + a_{12} \psi_2$$

$$\Phi_2(^4S) = a_{21} \psi_1 + a_{22} \psi_2$$

where

$$\psi_1 \equiv \Psi_1(1s 2p^3 [^5S] 2s \ ^4S)$$

$$\psi_2 \equiv \Psi_2(1s 2p^3 [^3S] 2s \ ^4S) \quad .$$

The amplitudes $|a_{11}| > |a_{12}|$ and $|a_{22}| > |a_{21}|$. These amplitudes and the eigenvectors are calculated within the framework of the perturbation theory. In order to distinguish such pairs they have been labeled with a subscript +(-) to indicate that the term has the higher (lower) value of the energy.

Another important point is the use of intermediate coupling scheme to calculate the decay of the metastable states. There are some terms, for example $1s2p^2\ ^4P$, which cannot decay radiatively or nonradiatively in the first order and in the LS-coupling scheme. However, this state can decay in the intermediate coupling scheme. The values of the total angular momentum are $J = \frac{1}{2}, \frac{3}{2},$ and $\frac{5}{2}$. There is a mixing of this state with other states with $J = \frac{1}{2}$, namely 2S and 2P terms of the same electronic configuration. The mixing coefficients are obtained by using the techniques outlined by Condon and Shortley²⁸, and then the rates are calculated.

A discussion of the results is presented in the next chapter.

TABLE IIa: Theoretical x-ray transition energies, E_x (in eV), lifetimes, τ (in sec), and multiplet partial fluorescence yields, $\omega(\alpha_{f_i} L_i S_i \rightarrow \alpha_{f_i} L_i S_i)$, for $2p^n$ configurations of fluorine.

Initial state		Final state	E_x	$\tau \times 10^{15}$	$\omega \times 100$
$2p$	$2p$	$1s$			
	$2S$	$2S$	827.4	242.41	100.00
$2p^2$		$1s 2p$			
	$1S$	$1P$	818.5	7.64	5.80
	$3P$	$3P$	813.9	134.10	100.00
	$1D$	$1P$	811.3	3.22	2.38
$2p^3$		$1s 2p^2$			
	$4S$	$4P$	797.7	100.00	100.00
	$2P$	$2S$	798.5	3.23	0.72
	$2P$	$2P$	809.0	3.23	1.68
	$2P$	$2D$	804.8	3.23	0.92
	$2D$	$2P$	804.5	2.39	1.23
	$2D$	$2D$	800.3	2.39	1.21
$2p^4$		$1s 2p^3$			
	$1S$	$1P$	791.4	1.90	2.34
	$3P$	$3S$	787.4	2.31	0.93
	$3P$	$3P$	786.9	2.31	0.70
	$3P$	$3D$	790.9	2.31	1.18
	$1D$	$1P$	784.9	1.50	0.45
	$1D$	$1D$	788.9	1.50	1.37
$2p^5$		$1s 2p^4$			
	$2P$	$2S$	775.6	1.36	0.12
	$2P$	$2P$	779.2	1.36	1.13
	$2P$	$2D$	781.2	1.36	0.63
$2p^6$		$1s 2p^5$			
	$1S$	$1P$	771.8	1.07	1.61

TABLE IIb: Theoretical x-ray transition energies, E_x (in eV), lifetimes, τ (in sec), and multiplet partial fluorescence yields, $\omega(\alpha_{L_i S_i \rightarrow f_f L_f S_f})$, for $2s2p^n$ configurations of fluorine.

Initial state	Final state	E_x	$\tau \times 10^{15}$	$\omega \times 100$
$2s2p$	$1s2s$			
1P	1S	811.4	63.76	21.82
3P	3S	806.9	64.00	21.53
$2s2p^2$	$1s2s2p$			
2S	$^2P_+$	802.6	4.98	0.38
2S	$^2P_-$	809.3	4.98	2.90
2P	$^2P_+$	804.8	4.45	2.55
2P	$^2P_-$	811.6	4.45	0.35
4P	4P	801.3	4.18	21.59
2D	$^2P_+$	795.7	2.80	0.21
2D	$^2P_-$	802.5	2.80	1.59
$2s2p^3$	$1s2s2p^2$			
3S	$^3P_+$	792.9	3.73	3.16
3S	$^3P_-$	803.7	3.73	0.18
5S	5P	789.2	24.89	21.87
1P	1S	793.1	2.14	0.42
1P	1P	792.9	2.14	0.95
1P	1D	799.1	2.14	0.54
3P	3S	787.7	2.84	0.55
3P	$^3P_+$	783.9	2.84	0.06
3P	$^3P_-$	794.7	2.84	1.21
3P	3D	793.7	2.84	0.70
1D	1P	788.6	1.79	0.78
1D	1D	794.8	1.79	0.80
3D	$^3P_+$	779.6	2.25	0.05
3D	$^3P_-$	790.4	2.25	0.96
3D	3D	789.3	2.25	0.99
$2s2p^4$	$1s2s2p^3$			
2S	$^2P_+$	778.3	1.65	0.22
2S	$^2P_-$	785.1	1.65	1.58

Initial State	Final state	E_x	$\tau \times 10^{15}$	$\omega \times 100$
2P	2S	780.2	1.64	0.59
2P	$^2P_+$	780.8	1.64	0.39
2P	$^2P_-$	787.6	1.64	0.06
2P	$^2D_+$	784.6	1.64	0.65
2P	$^2D_-$	791.4	1.64	0.10
4P	$^4S_+$	767.0	2.16	0.02
4P	$^4S_-$	782.0	2.16	0.75
4P	4P	777.2	2.16	0.57
4P	4D	781.0	2.16	0.97
2D	$^2P_+$	772.2	1.41	0.05
2D	$^2P_-$	778.9	1.41	0.33
2D	$^2D_+$	775.9	1.41	0.14
2D	$^2D_-$	782.7	1.41	1.00
$2s2p^5$	$1s2s2p^4$			
1P	1S	772.7	1.21	0.10
1P	1P	772.1	1.21	0.88
1P	1D	778.0	1.21	0.50
3P	3S	767.1	1.35	0.11
3P	$^3P_+$	763.1	1.35	0.05
3P	$^3P_-$	774.0	1.35	0.93
3P	3D	772.4	1.35	0.54
$2s2p^6$	$1s2s2p^5$			
2S	$^2P_+$	760.7	1.23	0.22
2S	$^2P_-$	767.4	1.23	1.42

TABLE IIc: Theoretical x-ray transition energies, E_x (in eV), lifetimes, τ (in sec), and multiplet partial fluorescence yields $\omega(\alpha_{L_i S_i} \rightarrow \alpha_{L_f S_f})$, for $2s^2 2p^n$ configurations of fluorine.

Initial state	Final state	E_x	$\tau \times 10^{15}$	$\omega \times 100$
$2s^2 2p$ 2P	$1s 2s^2$ 2S	805.2	4.03	1.28
$2s^2 2p^2$ 1S	$1s 2s^2 2p$ 1P	797.9	2.53	1.51
3P	3P	793.1	3.31	1.93
1D	1P	791.4	1.88	1.09
$2s^2 2p^3$ 4S	$1s 2s^2 2p^2$ 4P	782.5	5.31	4.25
2P	2S	780.5	1.80	0.32
2P	2P	782.3	1.80	0.73
2P	2D	786.2	1.80	0.41
2D	2P	780.2	1.57	0.62
2D	2D	782.0	1.57	0.63
$2s^2 2p^4$ 1S	$1s 2s^2 2p^3$ 1P	775.9	1.39	1.36
3P	3S	772.5	1.53	0.49
3P	3P	771.4	1.53	0.37
3P	3D	775.0	1.53	0.62
1D	1P	770.1	1.22	0.29
1D	1D	773.7	1.22	0.88
$2s^2 2p^5$ 2P	$1s 2s^2 2p^4$ 2S	762.4	1.16	0.08
2P	2P	765.8	1.16	0.76
2P	2D	767.3	1.16	0.42
$2s^2 2p^6$ 1S	$1s 2s^2 2p^5$ 1P	760.6	1.03	1.21

TABLE IIIa: Theoretical x-ray transition energies, E_x (in eV), lifetimes, τ (in sec), and multiplet partial fluorescence yields, $\omega(\alpha L_i S_i \rightarrow \alpha L_f S_f)$, for $1s^1 2p^n$ configurations of silicon.

Initial State	Final State	E_x	$\tau \times 10^{13}$	$\omega \times 100$
$1s 2p \begin{smallmatrix} 1 \\ 3 \end{smallmatrix} P$	$1s \begin{smallmatrix} 2 \\ 1 \end{smallmatrix} S$	1862.0	2.731(-1)	100.0
$\begin{smallmatrix} 3 \\ 3 \end{smallmatrix} P_1$	$1S$	1856.8	4.039(+3)	95.8
$\begin{smallmatrix} 3 \\ 3 \end{smallmatrix} P_2$	$1S$	1856.8	7.120(+4)	25.77
$1s 2p \begin{smallmatrix} 2 \\ 2 \end{smallmatrix} S$	$2P$	1854.6	3.223(-1)	48.89
$\begin{smallmatrix} 2 \\ 2 \end{smallmatrix} P$	$2P$	1847.0	2.014(-1)	99.83
$\begin{smallmatrix} 4 \\ 4 \end{smallmatrix} P_{1/2}$	$2P$	1831.8	4.416(+2)	99.85
$\begin{smallmatrix} 4 \\ 4 \end{smallmatrix} P_{3/2}$	$2P$	1831.8	1.096(+2)	28.45
$\begin{smallmatrix} 4 \\ 4 \end{smallmatrix} P_{5/2}$	$2P$	1831.8	1.831(+1)	10.97
$\begin{smallmatrix} 2 \\ 2 \end{smallmatrix} D$	$2P$	1844.0	6.649(-2)	11.06
$1s 2p \begin{smallmatrix} 3 \\ 3 \end{smallmatrix} S$	$1s \begin{smallmatrix} 2 \\ 2 \end{smallmatrix} P$	1826.3	1.600(-1)	100.0
$\begin{smallmatrix} 5 \\ 5 \end{smallmatrix} S_2$	$3P$	1807.1	4.422(+2)	10.71
$\begin{smallmatrix} 1 \\ 1 \end{smallmatrix} P$	$1S$	1822.2	5.488(-2)	11.36
$\begin{smallmatrix} 1 \\ 1 \end{smallmatrix} P$	$1D$	1832.1	5.488(-2)	14.43
$\begin{smallmatrix} 3 \\ 3 \end{smallmatrix} P$	$3P$	1829.0	6.626(-2)	10.40
$\begin{smallmatrix} 1 \\ 1 \end{smallmatrix} D$	$1D$	1825.2	4.331(-2)	20.27
$\begin{smallmatrix} 3 \\ 3 \end{smallmatrix} D$	$3P$	1822.2	5.010(-2)	7.78
$1s 2p \begin{smallmatrix} 4 \\ 2 \end{smallmatrix} S$	$1s \begin{smallmatrix} 2 \\ 2 \end{smallmatrix} P$	1810.7	3.656(-2)	10.72
$\begin{smallmatrix} 2 \\ 2 \end{smallmatrix} P$	$2P$	1803.3	3.877(-2)	8.42
$\begin{smallmatrix} 2 \\ 2 \end{smallmatrix} P$	$2D$	1809.6	3.877(-2)	14.19
$\begin{smallmatrix} 4 \\ 4 \end{smallmatrix} P$	$4S$	1805.4	4.669(-2)	6.79

TABLE IIIa: cont.

Initial State	Final State	E_x	$\tau \times 10^{13}$	$\omega \times 100$
2_D	2_P	1800.8	$2.945(-2)$	2.13
2_D	2_D	1807.1	$2.945(-2)$	6.44
$1s2p^5 1_P$	$1s^2 2p^4 1_S$	1782.1	$2.422(-2)$	2.17
1_P	1_D	1791.2	$2.422(-2)$	11.02
3_P	3_P	1788.7	$2.593(-2)$	7.06
$1s2p^6 2_S$	$1s^2 2p^5 2_P$	1773.5	$1.932(-2)$	7.33

TABLE IIIb: Theoretical x-ray transition energies, E_x (in eV), lifetimes, τ (in sec), and multiplet partial fluorescence yields, $\omega(\alpha_i L_i S_i \rightarrow \alpha_f L_f S_f)$, for $1s^1 2s^1 2p^n$ configurations of silicon.

Initial State	Final State	E_x	$\tau \times 10^{13}$	$\omega \times 100$
$1s2s \quad {}^3S^a$	$1s^2 \quad 1S$	1836.5	2.807(+7)	100.0
$1s2s2p \quad {}^2P^+$	$1s^2 2s \quad 2S$	1862.2	1.147(-1)	5.66
$2P^-$	$2S$	1854.1	2.599(-1)	74.37
$4P \quad 1/2$	$2S$	1835.6	6.831(+2)	68.46
$4P \quad 3/2$	$2S$	1835.6	2.523(+2)	67.60
$4P \quad 5/2^b$	$2S$	1835.6	1.844(+4)	7.09
$1s2s2p^2 \quad 1S$	$1s^2 2s2p \quad 1P$	1831.4	5.346(-2)	8.46
$3S$	$3P$	1383.2	1.197(-1)	19.16
$1P$	$1P$	1831.2	1.022(-1)	48.54
$3P^+$	$3P$	1843.5	7.242(-2)	1.71
$3P^-$	$3P$	1827.5	1.581(-1)	70.98
$5P \quad 1$	$3P$	1805.7	1.610(+2)	22.91
$5P \quad 2$	$3P$	1805.7	3.175(+2)	26.55
$5P \quad 3$	$3P$	1805.7	9.340(+1)	9.65
$1D$	$1P$	1821.1	3.825(-2)	5.96
$3D$	$3P$	1827.9	6.335(-2)	9.97
$1s2s2p^3 \quad 2S$	$1s^2 2s2p^2 \quad 2P$	1811.9	8.577(-3)	49.52
$4S^+$	$4P$	1829.7	1.007(-2)	0.95
$4S^-$	$4P$	1807.7	1.166(-1)	66.67
$6S \quad 5/2$	$4P$	1782.5	1.130(+2)	9.12

TABLE IIIb: cont.

Initial State	Final State	E_x	$\tau \times 10^{13}$	$\omega \times 100$
$2p_+$	$2s$	1814.5	$3.713(-2)$	0.88
$2p_+$	$2p$	1810.3	$3.713(-2)$	4.83
$2p_+$	$2d$	1824.0	$3.713(-2)$	1.11
$2p_-$	$2s$	1804.5	$4.079(-2)$	.71
$2p_-$	$2p$	1800.3	$4.079(-2)$	7.00
$2p_-$	$2d$	1814.0	$4.079(-2)$	8.89
$4p_-$	$4p$	1814.0	$6.442(-2)$	9.57
$2d_+$	$2p$	1803.7	$3.182(-2)$	4.09
$2d_+$	$2d$	1817.4	$3.182(-2)$	1.70
$2d_-$	$2p$	1793.7	$3.446(-2)$	.59
$2d_-$	$2d$	1807.4	$3.445(-2)$	13.38
$4d_-$	$4p$	1807.3	$4.994(-2)$	7.33
$1s2s2p^4 \ 1s$	$1s^2 2s2p^3 \ 1p$	1789.9	$2.192(-2)$	6.02
$3s$	$3p$	1797.0	$3.575(-2)$	9.93
$1p$	$1p$	1790.1	$3.411(-2)$	7.03
$1p$	$1d$	1796.2	$3.411(-2)$	11.83
$3p_+$	$3s$	1788.4	$2.527(-2)$	3.38
$3p_+$	$3p$	1802.5	$2.527(-2)$	.27
$3p_+$	$3d$	1808.6	$2.527(-2)$	.46
$3p_+$	$3s$	1772.1	$3.510(-2)$	.24
$3p_-$	$3p$	1786.2	$3.510(-2)$	6.81

TABLE IIIb: cont.

Initial State	Final State	E_x	$\tau \times 10^{13}$	$\omega \times 100$
$3P_-$	$3D$	1792.3	$3.510(-2)$	11.47
$5P$	$5S$	1791.6	$4.732(-2)$	6.51
$1D$	$1P$	1780.2	$1.934(-2)$	1.31
$1D$	$1D$	1786.3	$1.934(-2)$	3.96
$3D$	$3P$	1787.4	$2.935(-2)$	2.01
$3D$	$3D$	1793.5	$2.935(-2)$	6.08
$1s2s2p^5$	$1s^2 2s2p^4$			
$2P_+$	$2S$	1777.0	$1.672(-2)$	.18
$2P_+$	$2P$	1772.4	$1.672(-2)$	3.73
$2P_+$	$2D$	1785.7	$1.672(-2)$	.91
$2P_-$	$2S$	1766.8	$2.449(-2)$	1.80
$2P_-$	$2P$	1762.2	$2.449(-2)$	.77
$2P_-$	$2D$	1775.5	$2.449(-2)$	9.15
$4P$	$4P$	1776.2	$2.644(-2)$	6.79
$1s2s2p^6$	$1s^2 2s2p^5$			
$1S$	$1P$	1754.7	$1.385(-2)$	4.89
$3S$	$3P$	1762.1	$1.984(-2)$	7.09

^aG. W. F. Drake, Phys. Rev. A 3, 908 (1971).^bK. Cheng, C. Lin, W. R. Johnson, Phys. Lett. 48A, 437 (1974).

TABLE IIIc: Theoretical x-ray transition energies, E_x in (eV), lifetimes, τ (in sec), and multiplet partial fluorescence yields, $\omega(\alpha_L S_i \rightarrow \alpha_L S_i)$, for $1s^2 2s^2 2p^n$ configurations of silicon.

Initial State	Final State	E_x	$\tau \times 10^{13}$	$\omega \times 100$
$1s 2s^2 \ ^2S$	$1s^2 2p \ ^2P$	1806.4	8.240(-2)	1.42
$1s 2s^2 2p \ ^1P$	$1s^2 2s^2 \ ^1S$	1827.1	9.287(-2)	29.20
$3P$	$1S$	1822.2	7.494(-2)	0.0
$1s 2s^2 2p^2 \ ^2S$	$1s^2 2s^2 2p \ ^2P$	1819.7	4.712(-2)	7.10
$2P$	$2P$	1812.2	7.040(-2)	31.43
$4P$	$2P$	1798.3	5.668(-2)	0.0
$2D$	$2P$	1809.6	3.560(-2)	5.27
$1s 2s^2 2p^3 \ ^3S$	$1s^2 2s^2 2p^2 \ ^3P$	1793.8	5.919(-2)	32.96
$5S$	$3P$	1776.3	4.781(-2)	0.0
$1P$	$1S$	1790.2	3.396(-2)	6.26
$1P$	$1D$	1799.4	3.396(-2)	7.95
$3P$	$3P$	1796.8	3.179(-2)	4.45
$1D$	$1D$	1793.0	2.975(-2)	12.41
$3D$	$3P$	1790.3	2.808(-2)	3.89
$1s 2s^2 2p^4 \ ^2S$	$1s^2 2s^2 2p^3 \ ^2P$	1780.6	2.373(-2)	6.18
$2P$	$2P$	1773.4	2.728(-2)	5.27
$2P$	$2D$	1779.2	2.728(-2)	8.86
$4P$	$4S$	1775.7	2.547(-2)	3.29
$2D$	$2P$	1771.3	2.093(-2)	1.34

TABLE IIIc: cont.

Initial State	Final State	E_x	$\tau \times 10^{13}$	$\omega \times 100$
2_D	2_D	1777.2	2.093(-2)	4.07
$1s2s^2 2p^5 \ 1_P$	$1s^2 2s^2 2p^4 \ 1_S$	1754.8	1.931(-2)	1.53
1_P	1_D	1763.3	1.931(-2)	7.77
3_P	3_P	1761.2	1.878(-2)	4.52
$1s2s^2 2p^6 \ 2_S$	$1s^2 2s^2 2p^5 \ 2_P$	1748.1	2.338(-2)	7.81

TABLE IVa: Theoretical Auger rates, Γ_A (in a.u.), for different terms of the $1s2p^n$ configuration of fluorine leading to the various final terms. Initial and final states are designated by $|i\rangle = |\alpha_i L_i S_i\rangle$, and $|f\rangle = |\text{core (LS)} \epsilon l L_f S_f\rangle$, respectively.

$ i\rangle$	core (LS)	$\Gamma_A(i \rightarrow f)$
$1s2p^2$	$1s^2$	
2S	(^1S)	9.73
2D	(^1S)	24.50
$1s2p^3$	$1s^22p$	
1P	(^2P)	23.29
3P	(^2P)	23.29
1D	(^2P)	31.87
3D	(^2P)	31.87
$1s2p^4$	$1s^22p^2$	
2S	(^1S)	9.44
2S	(^1D)	30.00
2P	(^3P)	32.37
4P	(^3P)	32.37
2D	(^1S)	6.00
2D	(^1D)	44.37
$1s2p^5$	$1s^22p^3$	
1P	(^2P)	16.40
1P	(^2D)	37.56
3P	(^2P)	16.40
3P	(^2D)	37.56
$1s2p^6$	$1s^22p^4$	
2S	(^1S)	4.71
2S	(^1D)	61.45

TABLE IVb: Theoretical Auger rates, Γ_A (in a.u.), for different terms of the $1s2s2p^n$ configuration of fluorine leading to the various final terms. Initial and final states are designated by $|i\rangle = |\alpha_i L_i S_i\rangle$, and $|f\rangle = 1 \text{ core (LS)} \epsilon \alpha_f L_f S_f\rangle$, respectively.

$ i\rangle$	Core (LS)	Γ_A ($i \rightarrow f$)
$1s2p2s$	$1s^2$	
(1P) 2P	(1S)	2.07
(3P) 2P	(1S)	14.96
$1s2p^22s$	$1s^22p$	
1S	(2P)	22.66
3S	(2P)	2.86
1P	(2P)	8.57
(2P) 3P	(2P)	3.88
(4P) 3P	(2P)	24.50
1D	(2P)	22.66
3D	(2P)	2.86
	$1s^2 2s$	
1S	(2S)	8.62
3S	(2S)	8.62
1D	(2S)	21.70
3D	(2S)	21.70
$1s2p^32s$	$1s^22p^2$	
2S	(3P)	9.52
(3S) 4S	(3P)	5.64
(5S) 4S	(3P)	29.98
(1P) 2P	(1S)	1.02
2P	(3P)	12.03
2P	(1D)	1.27
(3P) 2P	(1S)	7.96
2P	(3P)	3.40
2P	(1D)	9.94
" 4P	(3P)	2.38
(1D) 2D	(3P)	12.03
2D	(1D)	2.29
(3D) 2D	(3P)	3.40
2D	(1D)	17.90

$ i\rangle$		Core (LS)	$\Gamma_A (i \rightarrow f)$
"	4D	$1s^2 2p^2 2s$	(^3P) 2.38
(^1P)	$^2P_-]$		(^1P) 0.53
	$^2P_-]$		(^3P) 19.73
(^3P)	$^2P_+]$		(^1P) 19.73
	$^2P_+]$		(^3P) 0.53
"	4P		(^3P) 20.26
(^1D)	$^2D]$		(^1P) 0.73
	$^2D]$		(^3P) 26.99
(^3D)	$^2D]$		(^1P) 26.99
	$^2D]$		(^3P) 0.73
"	4D		(^3P) 27.71
$1s 2p^4 2s$		$1s^2 2p^3$	(^2P) 33.76
	1S		(^2P) 3.93
	3S		(^2P) 2.95
	$^1P]$		(^2D) 4.91
	$^1P]$		(^4S) 4.01
(^2P)	$^3P]$		(^2P) 1.57
	$^3P]$		(^2D) 2.61
(^4P)	$^3P]$		(^4S) 7.89
	$^3P]$		(^2P) 8.84
	$^3P]$		(^2D) 14.73
"	5P	$1s^2 2p^2 2s$	(^4S) 1.97
	$^1D]$		(^2P) 8.44
	$^1D]$		(^2D) 25.32
	$^3D]$		(^2P) 0.98
	$^3D]$		(^2D) 2.95
	$^1S]$		(^2S) 7.98
	$^1S]$		(^2D) 25.67
	$^3S]$		(^2S) 7.98
	$^3S]$		(^2D) 25.67
	1P		(^2P) 27.67
(^2P)	$^3P_-]$		(^2P) 0.32

$ i\rangle$	Core (LS)	Γ_A (i→f)
(^4P)	$^3P \downarrow$	(^4P) 27.35
"	$^3P \downarrow$	(^2P) 27.35
"	$^3P \downarrow$	(^4P) 0.32
"	5P	(^4P) 27.67
"	$^1D \downarrow$	(^2S) 5.13
"	$^1D \downarrow$	(^2D) 37.93
"	$^3D \downarrow$	(^2S) 5.13
"	$^3D \downarrow$	(^2D) 37.93
$1s 2p^5 2s$	$1s^2 2p^4$	
(^1P)	$^2P \downarrow$	(^1S) 0.39
"	$^2P \downarrow$	(^3P) 2.65
"	$^2P \downarrow$	(^1D) 1.96
(^3P)	$^2P \downarrow$	(^1S) 2.80
"	$^2P \downarrow$	(^3P) 19.60
"	$^2P \downarrow$	(^1D) 14.01
"	4P	(^3P) 3.25
(^1P)	$1s^2 2p^3 2s$	
"	$^2P \downarrow$	(^1P) 0.35
"	$^2P \downarrow$	(^3P) 13.33
"	$^2P \downarrow$	(^1D) 0.80
"	$^2P \downarrow$	(^3D) 30.59
(^3P)	$^2P \downarrow$	(^1P) 13.33
"	$^2P \downarrow$	(^3P) 0.35
"	$^2P \downarrow$	(^1D) 30.59
"	$^2P \downarrow$	(^3D) 0.80
"	$^4P \downarrow$	(^3P) 13.68
"	$^4P \downarrow$	(^3D) 31.39
$1s 2p^6 2s$	$1s^2 2p^5$	
"	1S	(^2P) 36.11
"	3S	(^2P) 4.05
"	$1s^2 2p^4 2s$	
"	$^1S \downarrow$	(^2S) 3.84
"	$^1S \downarrow$	(^2D) 50.27
"	$^3S \downarrow$	(^2S) 3.84
"	$^3S \downarrow$	(^2D) 50.27

TABLE IVc: Theoretical Auger rates, Γ_A (in a.u.), for different terms of the $1s2s^22p^n$ configuration of fluorine leading to the various final terms. Initial and final states are designated by $|i\rangle = |\alpha_i L_i S_i\rangle$ and $|f\rangle = |\text{core (LS)} \epsilon L_f S_f\rangle$, respectively.

$ i\rangle$	Core (LS)	Γ_A (i→f)
$1s2s^2$	$1s^2$	
2S	(^1S)	19.27
$1s2s^22p$	$1s^2 2p$	
1P	(^2P)	14.44
3P	(^2P)	14.44
	$1s^2 2s$	
1P	(^2S)	0.02
3P	(^2S)	10.64
$1s2s^22p^2$	$1s^2 2p^2$	
2S	(^1S)	12.76
2P	(^3P)	12.76
4P	(^3P)	12.76
2D	(^1D)	12.76
	$1s^2 2s 2p$	
$^2S]$	(^1P)	10.55
$^2S]$	(^3P)	3.24
$^2P]$	(^1P)	3.24
$^2P]$	(^3P)	1.36
4P	(^3P)	18.38
$^2D]$	(^1P)	10.55
$^2D]$	(^3P)	3.24
	$1s^2 2s^2$	
2S	(^1S)	7.46
2D	(^1S)	18.84
$1s2s^22p^3$	$1s^2 2p^3$	
3S	(^4S)	11.06
5S	(^4S)	11.06
1P	(^2P)	11.06
3P	(^2P)	11.06
1D	(^2D)	11.06

$ i\rangle$	Core (LS)	$\Gamma_A(i \rightarrow f)$
3D	$1s^2 2s 2p^2$	(^2D) 11.06
3S		(^2P) 5.00
3S		(^4P) 2.78
5S		(^4P) 23.33
1P		(^2S) 0.002
1P		(^2P) 11.66
1P		(^2D) 0.002
3P		(^2S) 5.18
3P		(^2P) 5.28
3P		(^4P) 2.50
3P		(^2D) 6.48
1D		(^2P) 11.66
1D		(^2D) 0.004
3D		(^2P) 5.28
3D		(^4P) 2.50
3D		(^2D) 11.66
	$1s^2 2s^2 2p$	
1P		(^2P) 17.21
3P		(^2P) 17.21
1D		(^2P) 23.62
3D		(^2P) 23.62
$1s 2s^2 2p^4$	$1s^2 2p^4$	
2S		(^1S) 9.54
2P		(^3P) 9.54
4P		(^3P) 9.54
2D		(^1D) 9.54
	$1s^2 2s 2p^3$	
2S		(^1P) 14.76
2S		(^3P) 4.81
2P		(^3S) 8.70
2P		(^1P) 1.20
2P		(^3P) 0.43
2P		(^1D) 2.00
2P		(^3D) 0.71

$ i\rangle$	Core (LS)	$\Gamma_A(i \rightarrow f)$
$\left. \begin{array}{l} 4p \\ 4p \\ 4p \\ 4p \end{array} \right\}$	(^3S)	3.43
$\left. \begin{array}{l} 4p \\ 4p \\ 4p \end{array} \right\}$	(^5S)	2.00
$\left. \begin{array}{l} 4p \\ 4p \\ 4p \end{array} \right\}$	(^3P)	6.52
$\left. \begin{array}{l} 4p \\ 4p \\ 4p \end{array} \right\}$	(^3D)	10.87
$\left. \begin{array}{l} 2D \\ 2D \\ 2D \end{array} \right\}$	(^1P)	3.69
$\left. \begin{array}{l} 2D \\ 2D \\ 2D \end{array} \right\}$	(^3P)	1.20
$\left. \begin{array}{l} 2D \\ 2D \\ 2D \end{array} \right\}$	(^1D)	11.07
$\left. \begin{array}{l} 2D \\ 2D \\ 2D \end{array} \right\}$	(^3D)	3.61
$1s^2 2s^2 2p^2$		
$\left. \begin{array}{l} 2S \\ 2S \end{array} \right\}$	(^1S)	6.57
$\left. \begin{array}{l} 2S \\ 2S \end{array} \right\}$	(^1D)	21.35
$2P$	(^3P)	22.99
$4P$	(^3P)	22.99
$\left. \begin{array}{l} 2D \\ 2D \end{array} \right\}$	(^1S)	4.27
$\left. \begin{array}{l} 2D \\ 2D \end{array} \right\}$	(^1D)	31.53
$1s 2s^2 2p^5$	$1s^2 2p^5$	
$1P$	(^2P)	8.33
$3P$	(^2P)	8.33
$1s^2 2s 2p^4$		
$1P$	(^2S)	0.00
$\left. \begin{array}{l} 1P \\ 1P \end{array} \right\}$	(^2P)	16.31
$\left. \begin{array}{l} 1P \\ 1P \end{array} \right\}$	(^2D)	0.00
$\left. \begin{array}{l} 3P \\ 3P \end{array} \right\}$	(^2S)	1.81
$\left. \begin{array}{l} 3P \\ 3P \end{array} \right\}$	(^2P)	7.27
$\left. \begin{array}{l} 3P \\ 3P \end{array} \right\}$	(^4P)	3.61
$\left. \begin{array}{l} 3P \\ 3P \end{array} \right\}$	(^2D)	9.06
$1s^2 2s^2 2p^3$		
$1P$	(^2P)	11.09
$\left. \begin{array}{l} 1P \\ 1P \end{array} \right\}$	(^2D)	25.48
$\left. \begin{array}{l} 3P \\ 3P \end{array} \right\}$	(^2P)	11.09
$\left. \begin{array}{l} 3P \\ 3P \end{array} \right\}$	(^2D)	25.48

TABLE V: Theoretical average fluorescence yields multiplied by 100, $\omega \times 100$, for $1s2s^m2p^n$ configurations of various elements. The two numbers in parantheses (representing the range) are the minimum and the maximum values of the multiplet partial fluorescence yield for each configuration.

Configuration	$Z=7^a$	$Z=8^b$	$Z=9^c$	$Z=10^d$	$Z=14$
$1s2s^2$	0.09	0.15	0.29	0.38	1.42
$1s2s2p$	7.37	11.1	16.9	23.8	38.6
Range	(0.45-11.4)	(0.74-19.5)	(1.04-30.6)	(1.22-46.8)	(5.66-74.4)
$1s2p^2$	20.4	21.2	22.4	25.9	39.1
Range	(0.87-98.6)	(1.31-98.6)	(2.15-98.5)	(3.15-98.4)	(11.0-98.2)
$1s2s^22p$	0.57	0.99	1.58	2.39	7.30
Range	(0.0-2.29)	(0.0-3.94)	(0.0-632)	(0.0-9.57)	(0.0-29.2)
$1s2s2p^2$	4.19	7.17	6.60	14.8	21.9
Range	(0.12-9.48)	(0.20-16.5)	(0.32-26.3)	(0.48-35.5)	(1.71-71.0)
$1s2p^3$	7.77	8.29	9.64	10.8	18.5
Range	(0.56-100.0)	(0.83-100.0)	(1.13-100.0)	(2.19-100.0)	(7.78-100.0)
$1s2s^22p^2$	0.65		1.83	2.71	8.52
Range	(0.0-2.58)		(0.0-7.10)	(0.0-10.5)	(0.0-31.4)
$1s2s2p^3$	1.12	1.30	3.03	4.52	11.6
Range	(0.04-8.34)	(0.08-14.4)	(0.12-23.0)	(0.18-31.5)	(0.59-66.7)
$1s2p^4$		0.93	2.24	3.29	10.8
Range		(0.26-2.05)	(0.42-3.18)	(0.62-4.63)	(2.13-14.2)

TABLE V continued:

Configuration	Z=7	Z=8	Z=9	Z=10	Z=14
$1s2s^2 2p^3$	0.70	0.91	1.56	2.14	7.55
Range	(0.0-2.82)	(0.0-4.85)	(0.0-7.69)	(0.0-11.3)	(0.0-33.0)
$1s2s2p^4$		0.60	1.86	2.71	9.01
Range		(0.03-1.77)	(0.05-2.66)	(0.08-3.83)	(0.24-11.8)
$1s2p^5$			1.75	2.56	8.59
Range			(0.46-2.33)	(0.66-2.28)	(2.17-11.0)
$1s2s^2 2p^4$		0.53	1.27	1.87	6.36
Range		(0.17-1.18)	(0.26-1.86)	(0.39-2.69)	(1.34-8.86)
$1s2s2p^5$			1.57	2.35	7.53
Range			(0.04-1.93)	(0.05-3.09)	(0.18-9.15)
$1s2p^6$			1.30	2.24	7.38
$1s2s^2 2p^5$			1.17	1.09	5.71
Range			(0.32-1.64)	(0.47-2.33)	(1.53-7.77)
$1s2s2p^6$			1.41	2.02	6.54
Range			(1.02-1.54)	(1.43-2.21)	(4.89-7.09)
$1s2s^2 2p^6$			1.13	1.60	5.28

a) See reference 10

b) Unpublished work

c) See reference 14

d) See reference 8

CHAPTER IV

CONCLUSIONS

In this thesis detailed theoretical results for the atomic properties of various spectroscopic terms belonging to different electronic configurations of fluorine and silicon are presented. A brief description of the atomic model used in the calculations, and the relevant definitions are also given.

The multiplet partial fluorescence yield depends on the multiplicity and the orbital angular momentum ($2S + 1$, and L) value of a term for a specific configuration. The value of a particular multiplet partial fluorescence yield increases for increasing atomic number over the range of (N, O, F, Ne, and Si). When x-ray transition energies are compared for these elements, it is seen that the ordering of the multiplets for a particular configuration stays the same. For example, consider $2p \rightarrow 1s$ x-ray transitions for the initial terms of the electronic configuration $1s2s^2 2p^4$. The multiplets, in the order of increasing x-ray energy, are $^2D \rightarrow ^2P$, $^2P \rightarrow ^2P$, $^4P \rightarrow ^4S$, $^2D \rightarrow ^2D$, $^2P \rightarrow ^2D$, and $^2S \rightarrow ^2P$. It may be noted that the energy difference between two particular multiplets of this configuration, for instance $^2D \rightarrow ^2P$ and $^2P \rightarrow ^2P$, increases with increasing atomic number.

The average fluorescence yield, with the exception of the configurations $(1s2s^2 2p^n; n = 0 - 6)$, decreases as the number of electrons in the $2p$ subshell increases. The average fluorescence yield for $1s2s^2 2p^n$ configurations first increases, reaches its maximum for $n=2$, and then decreases.

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VITA

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THEORETICAL TRANSITION ENERGIES, LIFETIMES
AND FLUORESCENCE YIELDS FOR MULTIPLY-IONIZED
FLUORINE AND SILICON

by

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ABSTRACT

The Hartree-Fock-Slater model has been used to calculate the atomic properties of multiply-ionized fluorine and silicon. The numerical values for the x-ray transition energies, lifetimes, and multiplet partial fluorescence yields are presented for $(2s^m 2p^n)$ configurations of fluorine, and $(1s 2s^m 2p^n)$ configurations of silicon, and Auger rates for $(1s 2s^m 2p^n)$ configurations of fluorine. The multiplet factors for a large number of transitions were calculated and listed in this work.