RICE UNIVERSITY

EXCITED-STATE POPULATIONS OF SINGLY IONIZED SULPHUR IN GASEOUS NEBULAE

by

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ABSTRACT

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Jon C. Weisheit

A detailed study is made of the populations of singly ionized sulphur (SII) metastable states. These four states, $^2D_{3/2}$, $^2D_{5/2}$, $^2P_{1/2}$, $^2P_{3/2}$, and the ground state, $^4S_{3/2}$, arise from a $3p^3$ electron configuration.

Rates of populating the five states by collisional and radiative processes prominent in gaseous nebulae are examined. Inelastic electron-SII collision cross sections are estimated using a scaling technique suggested by Osterbrock (1965). The quantum defect method is used to calculate the photoionization cross sections of neutral and singly ionized sulphur.

With these and related data, population rate equations for all SII ($3p^3$) states are solved for numerous combinations of electron number densities and temperatures in the ranges $500 < N_e (\text{cm}^{-3}) < 10^9$; and $5,000 < T_e (\text{K}) < 30,000$. The number density ratio $N(^2D_{3/2})/N(^2D_{5/2})$, as a function of $N_e$ and $T_e$, is related to the intensity ratio of the forbidden transitions between $^2D_{3/2} - ^4S_{3/2} (\lambda 6717)$ and $^2D_{5/2} - ^4S_{3/2} (\lambda 6731)$. The results are used in conjunction with the intensity ratios observed in gaseous nebulae to obtain electron number densities in the regions of SII emission.

Finally, additional uses of SII spectra are noted.
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I. INTRODUCTION

The term gaseous nebula has been used by astronomers to denote celestial objects that cannot be resolved into stars. Among the objects included in this classification are planetary nebulae, the shells associated with novae events, and diffuse nebulae, such as Orion. Although the concepts discussed in this thesis apply to the various kinds of gaseous nebulae and even to other objects, for example HII regions and T-Tauri stars, emphasis is placed upon the study of planetary nebulae. These irradiated envelopes surrounding hot stars have been the subject of much observation and analysis. Their strong emission spectra reveal the presence of many ions (see TABLE V.1). Initial investigators - among them Bowen (1928), Ambarzumian (1933), and Wyse (1942) - soon realized that a large percentage of the lines were of unknown origin, and promptly began the task of identifying them.

More recently, theoretical efforts have been directed to problems involving the interpretation of line shapes and intensities; the present status of research pertaining to planetary nebulae is summarized by Aller and Middlehurst (1968). A short review article by Osterbrock (1964) also notes many of the problems that have arisen in the studies of nebular spectra. In particular, Osterbrock gives a succinct discussion of the HeI problem: the HeI (2^3S)
metastable state is being depopulated at a much faster rate than presently can be accounted for by known nebular processes. The problem is particularly imposing because the metastable state lies close to the upper bound states and the continuum; hence, even collisional or radiative processes involving only a little change in energy for the helium atom may be potentially important depopulation mechanisms.

This thesis is an investigation of the physical processes determining the intensities of singly ionized sulphur (SII) emission lines in gaseous nebulae. An SII term diagram is given in FIGURE I-1, and the corresponding energy splittings are listed in TABLE I.1. The data are from Moore (1949). Four metastable states arise from the ground \((3p^3)\) configuration: \(^2D_{3/2}, ^2D_{5/2}, ^2P_{1/2}, ^2P_{3/2}\). The forbidden transition lines from each of these states to the ground state, \(^4S_{3/2}\), have been detected in many nebulae. (These data are listed in TABLE V.1.) It should be noted that the five \((3p^3)\) states are well separated, energetically, from the upper excited states and the continuum. This situation isolates the slightly inelastic nebular events that are possible population and depopulation mechanisms.

Employing the appropriate transition probabilities (Einstein coefficients), one finds that the SII doublet levels are not populated according to Boltzmann's relation,
FIGURE I-1. A term diagram of singly-ionized sulphur showing the lower excited states. The level identifications are from Moore (1949).
SII TERM DIAGRAM

SII Ionization Potential = 23.4 ev.

FIGURE I-1
## TABLE 1.1
ENERGY LEVELS OF SINGLY IONIZED SULPHUR*

<table>
<thead>
<tr>
<th>Term</th>
<th>Wave Number (cm(^{-1}))</th>
<th>Excitation Energy (ev)</th>
</tr>
</thead>
<tbody>
<tr>
<td>3p (^1S_{3/2})</td>
<td>188 824.5</td>
<td>0</td>
</tr>
<tr>
<td>3p (^2D_{3/2})</td>
<td>173 972.6</td>
<td>1.841</td>
</tr>
<tr>
<td>3p (^2D_{5/2})</td>
<td>173 941.1</td>
<td>1.845</td>
</tr>
<tr>
<td>3p (^2P_{1/2})</td>
<td>164 300.3</td>
<td>3.040</td>
</tr>
<tr>
<td>3p (^2P_{3/2})</td>
<td>164 251.7</td>
<td>3.046</td>
</tr>
<tr>
<td>4s (^2P_{1/2})</td>
<td>75 887.17</td>
<td>14.002</td>
</tr>
<tr>
<td>4s (^2P_{3/2})</td>
<td>75 363.28</td>
<td>14.066</td>
</tr>
<tr>
<td>3d (^2F_{5/2})</td>
<td>74 020.39</td>
<td>14.232</td>
</tr>
<tr>
<td>3d (^2F_{3/2})</td>
<td>73 539.19</td>
<td>14.293</td>
</tr>
<tr>
<td>3d (^2P_{3/2})</td>
<td>70 678.00</td>
<td>14.648</td>
</tr>
<tr>
<td>3d (^2D_{3/2})</td>
<td>69 582.37</td>
<td>14.783</td>
</tr>
<tr>
<td>3d (^2D_{5/2})</td>
<td>69 529.80</td>
<td>14.790</td>
</tr>
</tbody>
</table>

*from Moore (1949)
\( \frac{N_i}{N_j} = \left( \frac{\omega_i}{\omega_j} \right) e^{-\frac{(E_j - E_i)}{kT}} \)  \hspace{1cm} (1.1)

N, \( \omega \), and E are the number density, statistical weight, and energy, respectively, of a given state.

To explain the deviations from thermodynamic equilibrium abundances, one must determine the rates of populating and depopulating these states. Since nebular spectra appear to be constant (with respect to time), a steady-state condition exists. The total rate of populating a state, consequently, must equal its total rate of depopulation.

The following two sections are devoted to the calculation of collisional and radiative rates of population for all five of the SII(3p^3) levels. Subsequently, steady-state (equilibrium) abundance equations are solved, and the sensitivity of the solutions, \( \frac{N(\text{SII excited state})}{N(\text{SII ground state})} \), to changes in various nebular parameters, i.e. electron number density and temperature, is examined.
II. COLLISIONAL PROCESSES

To establish the possibility of inelastic collisional processes being important depopulation mechanisms for the states of SII under consideration, one needs to compare their radiative lifetimes to collision times.

The radiative lifetime, $t_x$, of a given state (x) may be expressed

$$t_x = \left[ \sum_y A_{xy} \right]^{-1} \tag{2.1}$$

where $A_{xy}$ is the transition probability (sec$^{-1}$) for the radiative decay of state (x) to state (y), and the sum is over all lower-lying states. The time $\tau$ between collisions can be obtained from a kinetic argument (Huang, 1963) as follows: consider a system of two types of particles, each having an equilibrium distribution function $f_i(\vec{r}_i, \vec{v}_i, t)$, and a number density $n_i$. The number of collisions per second per unit volume is given by

$$Y = \int d\vec{v}_1 \int d\vec{v}_2 \int d\Omega \sigma(\Omega) |\vec{v}_1 - \vec{v}_2| f_1(\vec{r}_1, \vec{v}_1, t) f_2(\vec{r}_2, \vec{v}_2, t) \tag{2.2}$$

$\sigma(\Omega)d\Omega$ is the differential cross section for the collision of two different kinds of particles. Transforming to center-of-mass coordinates, and performing the angular integral, Equation (2.2) reduces to

$$Y = \int d^3V \int d^3V \sigma \cdot v \cdot n_1 \cdot n_2 \frac{m_1}{2\pi kT} \frac{m_2}{2\pi kT} \exp \left[ - \frac{MV^2 + UV^2}{2kT} \right] \tag{2.3}$$
the notation being \( \sigma = \int d\Omega \sigma(\Omega) \), \( M = m_1 + m_2 \), \( \mu = \frac{m_1 m_2}{m_1 + m_2} \),

\[
V = \frac{m_1 \vec{v}_1 + m_2 \vec{v}_2}{m_1 + m_2} \quad \text{and} \quad v = |\vec{v}_1 - \vec{v}_2|.
\]

If \( \sigma \) is not sensitive to the energy of the colliding particles, the expression for \( Y \) becomes

\[
Y = n_1 n_2 \sigma \left( \frac{4}{\pi} \frac{2kT}{\mu} \right)^{1/2},
\]

and recognizing \( \left( \frac{2kT}{\mu} \right)^{1/2} \) as an average thermal speed, \( \langle v \rangle \), one can write

\[
Y = 2\pi^{-1/2} n_1 n_2 \sigma \langle v \rangle \frac{\text{collisions}}{\text{unit vol.-unit time}} \quad (2.4)
\]

The collision time for particles of type (x) is defined by

\[
\tau_x = \frac{n_x}{Y} \text{ sec.} \quad (2.5)
\]

Employing typical nebular values, \( T(\text{electron}) = 10^4 \)°K, \( n = 10^4 / \text{cm}^3 \), one finds that cross sections at least as large as \( (10^{-12} / \tau_x) \) cm\(^2\) are required for ion-electron collisions to contribute significantly to the depopulation of the ionic state. Because of the mass difference of ions and electrons and the lower ionic number densities in nebulae, it is evident from Equations (2.4) and (2.5) that ion-ion collisions need not be considered for the rate of depopulation of excited states of ions unless the ion-ion cross section is 100 times larger than the ion-electron cross section.

Under conditions existing in gaseous nebulae photon-ion collisions might also be important inelastic processes for depopulating states with large lifetimes— metastable
and ground states. Since one-photon processes are generally more probable than two-photon processes, (ignoring infrequent resonance excitations) photoionization is the most likely photo-absorption event. The rate of state \((x)\) being photoionized to state \((y)\) is

\[
\psi_{xy} = N_x \int \frac{4\pi I_v \alpha_{xy}(v)}{h \nu} \, dv \, \text{cm}^{-3} \text{sec}^{-1} \tag{2.6}
\]

where \(\alpha_{xy}(v)\) = photoionization cross section: \((x)\rightarrow(y)\)

\(\nu = \text{photon frequency}\)

\(I_v dv = \text{Bose-Einstein distribution function for the intensity of incident photons (ergs/cm}^2 \cdot \text{sec) in the interval} \, dv.\)

Equation (2.6) is readily obtained from Equation (2.2) by substituting the appropriate (photon) distribution function and then performing the angular integral and the integral over the particle's velocity. As before, \(N_x/\psi_{xy}\) must be comparable to the lifetime of the initial state \((x)\) if photoionization is to be a significant depopulation mechanism. Although the inelastic collisions of electrons and ions cause departures from equilibrium in the populations of excited states, Coulombic encounters between the charged particles occur with such frequency that velocity distribution functions quickly approach equilibrium. Spitzer (1962) obtains the relation

\[
\tau_r = \frac{m \nu^2 (3kT)^{3/2}}{8 \times 0.714 \pi ne^4 Z^4 \ln A} = \frac{11.4 A^{1/2} \tau^{3/2}}{nZ^4 \ln A} \, \text{sec.} \tag{2.7}
\]
for the relaxation time in an ionized gas. \( n, Z, \) and \( A \)
are the number density, charge, and atomic number of ions
under consideration at a temperature \( T. \) \( A \) is a complicated
function of \( T \) and \( n, \) and is tabulated by Spitzer. For
electrons in an average nebular environment,

\[ t_r(\text{electrons}) = 1.5 \text{ sec.} \quad (2.8) \]

A more elaborate discussion of this topic is given by Bohm
and Aller (1947). For metastable states \( \tau \) is typically of
the order of \( 10^3 \) sec, indicating that for such cases the
electrons reach equilibrium almost immediately after an
inelastic event.

The concepts discussed above indicate that inelastic
electron-ion and photon-ion events constitute essentially
all of the collisional depopulation mechanisms in gaseous
nebulae. The remainder of this section is devoted to exam-
inig these processes.
A. Rates for Inelastic Electron-SII Collisions

The pertinent inelastic events are those in which the initial and final states of SII are among $^4S$, $^2D$, and $^2P$. The cross section for excitation of the j$^\text{th}$ term from the i$^\text{th}$ term can be expressed [See Appendix A for a more detailed treatment of the inelastic cross sections discussed here.]

$$Q(i,j) = \frac{\pi}{k^2 \omega_i} \Omega(i,j)$$  \hspace{1cm} (2.9)

where $\omega_i$ is the degeneracy of the initial term, and the wave number of the incident electron $k$ is its momentum divided by $\hbar$. $\Omega(i,j)$ is a dimensionless quantity called the collision strength, or target area parameter, and is not strongly energy-dependent.

By Equation (2.9), the rate of collisional excitation of state (j) due to electrons colliding with atoms in state (i) is

$$Y_{ij} = N_i N_e \int Q(i,j) v f(v) dv$$

$$= N_i N_e \frac{\pi}{\omega_i} \left(\frac{\hbar}{mv}\right)^2 \Omega(i,j) v f(v) dv$$  \hspace{1cm} (2.10)

For a Maxwellian distribution of electron velocities and a constant $\Omega$, integration from $v = v_0$ to $v = \infty$ gives

$$Y_{ij} = 8.63 \times 10^{-6} \frac{N_i N_e}{\omega_i T_e^{\frac{3}{2}}} \Omega(i,j) e^{-E_{ji}/kT_e} \text{ cm}^{-3} \text{ sec}^{-1}$$  \hspace{1cm} (2.11)

$1/2 \,mv_0^2 = E_{ji}$, the threshold energy for the collision; $T_e$ is
the kinetic temperature of the electrons. From balancing collisional rates in thermodynamic equilibrium,

\[ \Omega(i,j) = \Omega(j,i) \]  \hspace{1cm} (2.12)

Calculations of collision strengths for specific transitions, viz. \( \Omega(\text{LSJ}+\text{L'S}'\text{J}') \), are quite difficult. More easily obtained are \( \Omega \)'s for transitions between terms, (\( \text{LS}+\text{L'S}' \)). In fact, only for OII (2p\(^3\)) have the former been evaluated directly [Seaton, 1958]. Since SII has a similar configuration, 3p\(^3\), the following scheme was used to obtain the desired SII collision strengths:

\[ \Omega_{\text{SII}}(\text{LSJ}+\text{L'S}'\text{J}') = \frac{\Omega_{\text{OII}}(\text{LSJ}+\text{L'S}'\text{J}') \Omega_{\text{SII}}(\text{LS}+\text{L'S}')}{\Omega_{\text{OII}}(\text{LS}+\text{L'S}')} \] \hspace{1cm} (2.13)

Equation (2.13) is also derivable from the approximation suggested by the data of Hebb and Menzel (1940), and used by many authors,

\[ \Omega(\text{LSJ}+\text{L'S}'\text{J}') = \frac{(2J+1)(2J'+1)}{(2L+1)(2L'+1)(2S+1)(2S'+1)} \Omega(\text{LS}+\text{L'S}') \] \hspace{1cm} (2.14)

From this expression, the ratios

\[ \frac{\Omega(4S,2D_{5/2})}{\Omega(4S,2D_{3/2})} = \frac{2}{3} = \frac{\omega(2D_{3/2})}{\omega(2D_{5/2})} \]

and

\[ \frac{\Omega(4S,2P_{1/2})}{\Omega(4S,2P_{3/2})} = \frac{1}{2} = \frac{\omega(2P_{1/2})}{\omega(2P_{3/2})} \] \hspace{1cm} (2.15)

result, in agreement with the analytic work of Seaton (1958).
For the transitions $^2D_{3/2} \leftrightarrow ^2D_{5/2}$ and $^2P_{3/2} \leftrightarrow ^2P_{3/2}$, however, Equations (2.13) and (2.14) do not apply: $\Omega(\text{LS} \leftrightarrow \text{LS})$ have not been defined in the context in which collision strengths are used here.

The $^2D \leftrightarrow ^2P$ transition does not involve a change of multiplicity, whereas the $^4S \leftrightarrow ^2D$, $^2P$ transitions do. Moiseiwitsch and Smith (1968) have pointed out that, as a consequence, $\Omega(^4S; ^2D_{3/2}, ^2D_{5/2})$ and $\Omega(^4S; ^2P_{3/2}, ^2P_{3/2})$ depend entirely upon exchange coupling between the initial and final states; $\Omega(^2D_{3/2}, ^2P_{3/2}; ^2P_{3/2}, ^2P_{3/2})$, though, depend upon both exchange and potential coupling. With this information, a scaling technique suggested by Osterbrock (1965) can be employed to evaluate the collision strengths $\Omega(^2P_{3/2}, ^2P_{3/2})$ and $\Omega(^2P_{3/2}, ^2D_{5/2})$, which also depend upon both types of coupling. The appropriate expressions are:

$$\Omega_{\text{SII}}(^2D_{3/2}, ^2D_{5/2}) = \Omega_{\text{OII}}(^2D_{3/2}, ^2D_{5/2}) \frac{\Omega_{\text{SII}}(^2D, ^2P)}{\Omega_{\text{OII}}(^2D, ^2P)}$$

$$\Omega_{\text{SII}}(^2P_{3/2}, ^2P_{3/2}) = \Omega_{\text{OII}}(^2P_{3/2}, ^2P_{3/2}) \frac{\Omega_{\text{SII}}(^2D, ^2P)}{\Omega_{\text{OII}}(^2D, ^2P)}$$

Equations (2.13) and (2.16) are used to obtain the SII collision strengths needed. The calculated values are listed in TABLE II.1; the pertinent OII collision strengths of Seaton and SII collision strengths of Czyzak and Krueger (1967) are also given.

From Equation (2.11) and the data of TABLE II.1, a
collision rate coefficient for a particular electron temperature, \((Y_{ij}/N_e N_i) = R_{ij}\), can be calculated. Choosing temperatures 5,000°K - 30,000°K, a range that should include most nebular values, collision rate coefficients are tabulated in TABLE II.2. The collision strengths given here were varied by ±25% (see Section IV) and the sensitivity of the solution of the rate equations to these variances is noted.
### TABLE II.1
OII AND SII COLLISION STRENGTHS

<table>
<thead>
<tr>
<th>COLLISION STRENGTH</th>
<th>OXYGEN II</th>
<th>SULPHUR II</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\Omega(^4S,^2D)$</td>
<td>1.28 *</td>
<td>3.07 **</td>
</tr>
<tr>
<td>$\Omega(^4S,^2P)$</td>
<td>0.58 *</td>
<td>1.28 **</td>
</tr>
<tr>
<td>$\Omega(^2D,^2P)$</td>
<td>2.12 *</td>
<td>6.22 **</td>
</tr>
<tr>
<td>$\Omega(^4S,^2D_{3/2})$</td>
<td>0.51 *</td>
<td>1.2</td>
</tr>
<tr>
<td>$\Omega(^4S,^2D_{5/2})$</td>
<td>0.77 *</td>
<td>1.8</td>
</tr>
<tr>
<td>$\Omega(^4S,^2P_{1/2})$</td>
<td>0.19 *</td>
<td>0.43</td>
</tr>
<tr>
<td>$\Omega(^4S,^2P_{3/2})$</td>
<td>0.39 *</td>
<td>0.86</td>
</tr>
<tr>
<td>$\Omega(^2D_{3/2},^2P_{1/2})$</td>
<td>0.33 *</td>
<td>0.97</td>
</tr>
<tr>
<td>$\Omega(^2D_{3/2},^2P_{3/2})$</td>
<td>0.52 *</td>
<td>1.5</td>
</tr>
<tr>
<td>$\Omega(^2D_{5/2},^2P_{1/2})$</td>
<td>0.38 *</td>
<td>1.1</td>
</tr>
<tr>
<td>$\Omega(^2D_{5/2},^2P_{3/2})$</td>
<td>0.89 *</td>
<td>2.6</td>
</tr>
<tr>
<td>$\Omega(^2D_{3/2},^2D_{5/2})$</td>
<td>0.85 *</td>
<td>2.5</td>
</tr>
<tr>
<td>$\Omega(^2P_{1/2},^2P_{3/2})$</td>
<td>0.33 *</td>
<td>0.97</td>
</tr>
</tbody>
</table>

*Seaton (1958)

** Czyzak and Krueger (1967)
TABLE II.2
SULPHUR II COLLISION RATE COEFFICIENTS

<table>
<thead>
<tr>
<th>$R_i \rightarrow j$</th>
<th>$T_4 = 0.5$</th>
<th>$T_4 = 1.0$</th>
<th>$T_4 = 1.5$</th>
<th>$T_4 = 3.0$</th>
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</thead>
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<tr>
<td>$R_{12}$</td>
<td>0.0510</td>
<td>0.306</td>
<td>0.509</td>
<td>0.733</td>
</tr>
<tr>
<td>$R_{13}$</td>
<td>0.0759</td>
<td>0.456</td>
<td>0.761</td>
<td>1.10</td>
</tr>
<tr>
<td>$R_{14}$</td>
<td>0.00113</td>
<td>0.0272</td>
<td>0.0721</td>
<td>0.165</td>
</tr>
<tr>
<td>$R_{15}$</td>
<td>0.00223</td>
<td>0.0541</td>
<td>0.144</td>
<td>0.330</td>
</tr>
<tr>
<td>$R_{21}$</td>
<td>3.66</td>
<td>2.59</td>
<td>2.11</td>
<td>1.49</td>
</tr>
<tr>
<td>$R_{23}$</td>
<td>7.56</td>
<td>5.37</td>
<td>4.39</td>
<td>3.11</td>
</tr>
<tr>
<td>$R_{24}$</td>
<td>0.183</td>
<td>0.521</td>
<td>0.676</td>
<td>0.760</td>
</tr>
<tr>
<td>$R_{25}$</td>
<td>0.279</td>
<td>0.799</td>
<td>1.04</td>
<td>1.17</td>
</tr>
<tr>
<td>$R_{31}$</td>
<td>3.66</td>
<td>2.59</td>
<td>2.11</td>
<td>1.49</td>
</tr>
<tr>
<td>$R_{32}$</td>
<td>5.09</td>
<td>3.60</td>
<td>2.94</td>
<td>2.08</td>
</tr>
<tr>
<td>$R_{34}$</td>
<td>0.140</td>
<td>0.395</td>
<td>0.512</td>
<td>0.575</td>
</tr>
<tr>
<td>$R_{35}$</td>
<td>0.326</td>
<td>0.928</td>
<td>1.21</td>
<td>1.37</td>
</tr>
<tr>
<td>$R_{41}$</td>
<td>2.62</td>
<td>1.86</td>
<td>1.51</td>
<td>1.07</td>
</tr>
<tr>
<td>$R_{42}$</td>
<td>5.92</td>
<td>4.19</td>
<td>3.42</td>
<td>2.42</td>
</tr>
<tr>
<td>$R_{43}$</td>
<td>6.71</td>
<td>4.75</td>
<td>3.88</td>
<td>2.74</td>
</tr>
<tr>
<td>$R_{45}$</td>
<td>5.84</td>
<td>4.16</td>
<td>3.40</td>
<td>2.41</td>
</tr>
<tr>
<td>$R_{51}$</td>
<td>2.62</td>
<td>1.86</td>
<td>1.51</td>
<td>1.07</td>
</tr>
<tr>
<td>$R_{52}$</td>
<td>4.58</td>
<td>3.24</td>
<td>2.64</td>
<td>1.87</td>
</tr>
<tr>
<td>$R_{53}$</td>
<td>7.93</td>
<td>5.61</td>
<td>4.58</td>
<td>3.24</td>
</tr>
<tr>
<td>$R_{54}$</td>
<td>2.96</td>
<td>2.09</td>
<td>1.71</td>
<td>1.21</td>
</tr>
</tbody>
</table>

The coefficients $R_{ij}$ are in units $10^{-8} \text{cm}^3\text{sec}^{-1}$. 
$T_4 = T^{(\circ K)} \times 10^{-4}$.

$1 \rightarrow ^4S_{3/2}$; $2 \rightarrow ^2D_{3/2}$; $3 \rightarrow ^2D_{5/2}$; $4 \rightarrow ^2P_{1/2}$; $5 \rightarrow ^2P_{3/2}$.
B. Photoionization Rates of SI and SII

As discussed earlier, a photoionization rate may be written as

\[ \psi_{xy} = N_x \frac{4\pi I_x \alpha_{xy}(\nu)}{h\nu} \, d\nu \, \text{cm}^{-3} \text{sec}^{-1}. \]  

(2.17)

If the ejected electron has an energy \( Z^2\epsilon \), \( Z \) being the residual charge of the ion, and \( \chi_x \) is the ionization potential,

\[ h\nu = \chi_x + Z^2\epsilon. \]  

(2.18)

The photon distribution function is taken to be representable by a thermal spectrum having diluted energy density

\[ I_\nu \, d\nu = W \frac{2h\nu^3}{c^2} \left( e^{h\nu/kT_\nu} - 1 \right)^{-1} \, d\nu. \]  

(2.19)

\( W \) is the dilution factor.

In Rydberg units, 1 Ryd = 13.605 ev = 2.180x10^-11 erg, Equation (2.17) can be rewritten as an integral over the ejected electron's energy:

\[ \chi_{xy} = \frac{8\pi N_x}{c^2h^3} \int_0^\infty \frac{(\chi_x + Z^2\epsilon)^2 \alpha_{xy}(\epsilon)}{W \left[ e^{(\chi_x+Z^2\epsilon)/kT_\nu} - 1 \right]} \, d(Z^2\epsilon) \]

\[ = 9.94 \times 10^{26} N_x Z^2 \int_0^\infty \frac{(\chi_x + Z^2\epsilon)^2 \alpha_{xy}(\epsilon)}{W \left[ e^{(\chi_x+Z^2\epsilon)/kT_\nu} - 1 \right]} \, d\epsilon. \]  

(2.20)

Boltzmann's constant is in Rydberg units, \( k = 6.33 \times 10^{-6} \) Ryd/°K.

In collisional equilibrium, \( T_\nu = T_e = T \). However, as emphasized throughout this thesis, this condition does not
exist in gaseous nebulae. The question then arises as to the relation between $T_v$ and $T_e$. Aller (1938) pointed out that as the temperature of the central star increases so does the electron temperature - but the increase is much more gradual. A primary reason is that excitation of an atomic metastable state decreases the incident electron's energy, and subsequent forbidden line radiation, which escapes the nebulae, does not return this energy to the electron gas. [For further details on this point, see Hjellming, 1966.] In the (1938) article Aller discusses a nebula in which radiative processes dominate. Energy conservation considerations led him to a functional relation between $T_e$ and $T_v$. For the case of an optically thin, purely hydrogenic nebula, Aller obtained the numerical results given in TABLE II.3.

The expression

$$T_v \left( \text{radiative} \right) = T_e \left( 1 + \frac{1}{12} \ln \frac{T_e}{5000} \right)$$

represents the Aller data in the region of interest, $T_e < 50,000^\circ K$, to within 10%.

The physical state of a nebula is somewhere between the extremes of an equilibrium dominated by radiative processes and one dominated by collisional processes. It seems reasonable, then, that in a first approximation,
\[ T_v = \frac{1}{2} \left[ T_v^{\text{radiative}} + T_v^{\text{collisional}} \right] \]

\[ = \frac{1}{2} \left[ T_v^{\text{equilibrium}} + T_e \right] \quad (2.22) \]

From 2.21 and 2.22 the desired relation is obtained:

\[ T_v = T_e + \frac{T_e}{24} \ln \left( \frac{T_e}{5000} \right), \quad T_e < 50,000^\circ K \quad (2.23) \]
"Theoretical Relation between the Electron Temperature and the Temperature of the Central Star for a Thin Nebula consisting of pure hydrogen"*

<table>
<thead>
<tr>
<th>Temperature of Central Star</th>
<th>Electron Temperature</th>
</tr>
</thead>
<tbody>
<tr>
<td>$T_v$</td>
<td>$T_e$</td>
</tr>
<tr>
<td>$5,000^\circ K$</td>
<td>$9,500$</td>
</tr>
<tr>
<td>10,000</td>
<td>18,000</td>
</tr>
<tr>
<td>20,000</td>
<td>34,000</td>
</tr>
<tr>
<td>40,000</td>
<td>57,000</td>
</tr>
<tr>
<td>80,000</td>
<td>92,000</td>
</tr>
<tr>
<td>160,000</td>
<td>132,000</td>
</tr>
</tbody>
</table>

*from Aller (1938)
C. **Radiative Dilution Factor**

The intensity of radiation impinging upon ions in any given nebular volume element a distance \( r \) from a central star of radius \( R \) is diluted by the geometrical factor \( \frac{R^2}{r^2} \). Moreover, the matter between the star and the volume element under consideration absorbs and reradiates the photons incident upon it. This process tends to degrade the more energetic quanta. The volume element also receives radiation back-scattered from more distant elements, so that even if the initial stellar spectrum were well defined - say, that of a black body - the photon spectrum that irradiates a particular volume element is more complicated.

Since these radiative events are not well understood quantitatively, the intensity of incident photons can only be approximated. A great simplification results if the dilution of radiation is taken independent of frequency, and assigned a value determined solely by the geometry of the nebula. The problems associated with more exact treatments of radiation dilution are discussed by Menzel and Aller (1941). These authors also calculated numerous mean geometrical dilution factors and obtained \( 10^{-15} \leq \bar{W} \leq 10^{-14} \), depending upon the nebula chosen. This \( \bar{W} \) is taken to be \( \frac{1}{4} \frac{R^2}{\bar{r}^2} \), where \( \bar{r} \) is the mean radius of the nebular emission envelope.

In this thesis, values of 1, 5, and \( 10 \times 10^{-15} \) are given
to $\bar{W}$ and the sensitivity of various results to the specific number used is noted. The above approximation simplifies Equation (2.20) so that

$$\psi_{xy} = 9.94 \times 10^{2.6} N_x Z^2 \bar{W} \int_0^\infty \frac{(x_x + Z^2 \varepsilon)^2 a_{xy}(\varepsilon)}{e^{(x_x + Z^2 \varepsilon)/kT_x} - 1} \, d\varepsilon.$$
D. Photoionization Cross Sections for SI and SII

The approach used here to calculate the photoionization cross sections of neutral and singly ionized sulphur is due to Burgess and Seaton (1960a). The technique is a quantum defect method, wherein asymptotic forms for the continuum states of the atomic system* are obtained from bound-state energy levels of the atom. The quantum defect of an atomic system is briefly discussed, and then the Burgess and Seaton quantum defect method (QDM) is used to obtain photoionization cross sections for these transitions:

\[
\begin{align*}
SI(3P) + \gamma &\rightarrow SII(4S) + e^- \\
SI(3P) + \gamma &\rightarrow SII(2D) + e^- \\
SI(3P) + \gamma &\rightarrow SII(2P) + e^- \\
SII(4S) + \gamma &\rightarrow SIII(3P) + e^- \\
SII(2D) + \gamma &\rightarrow SIII(3P) + e^- \\
SII(2D) + \gamma &\rightarrow SIII(1D) + e^- \\
SII(2P) + \gamma &\rightarrow SIII(3P) + e^- \\
SII(2P) + \gamma &\rightarrow SIII(1D) + e^- \\
SII(2P) + \gamma &\rightarrow SIII(1S) + e^- \\
\end{align*}
\]

The general theory of photoionization is reviewed in Appendix B.

*Hereafter, "atomic system" refers to the initial system which can, of course, be an ion.
1. The Quantum Defects of SI and SII

The consideration of many atomic phenomena in which two or more systems interact requires evaluation of matrix elements between initial and final states: \( \langle \text{final} | V_{\text{int}} | \text{initial} \rangle \). Often the wave functions are not accurately known, making it impossible to calculate the matrix element directly. In some instances, an alternate approach is to use the quantum defect method. The QDM, as noted above, obtains asymptotic expressions for atomic wave functions. The utility of such a procedure is demonstrated by the following pertinent example. Consider an ionizing collision; the final state is that of a continuum electron plus the ion. If the ejected electron's kinetic energy is small the system can be likened to the initial atom with an outer electron having positive binding energy. The QDM obtains an asymptotic wave function for the ejected electron by a process of analytic continuation, the formalities of which have been given by Ham (1955) and Seaton (1958).

If \( n, L, \) and \( S \) are the principal, orbital angular momentum, and spin angular momentum quantum numbers, respectively, of a bound electron with energy

\[
E_{nLS} = -\frac{(ZZ'e^2)m}{2\hbar^2(v')^2} = -\frac{Z^2}{(v')^2} \text{ Ryd},
\]

the quantum defect \( \mu_{nLS} \) is defined by

\[
\mu_{nLS} = n - v'
\]
so that, for an exact Coulomb potential, \( \mu = 0 \). Expressed as a function of binding energy

\[
\mu_{nLS}(E_{nLS}) = n - (Z^2/E_{nLS})^{1/2}
\]  

(2.24)

In theory, the quantum defect varies smoothly as the binding energy goes from negative (bound state) to positive (continuum state). But in application it is found that very small (~10 cm\(^{-1}\)) deviations in the binding energy can produce large errors in the quantum defect. This problem is discussed in some detail by Goldwire (1967).

Because such uncertainties make accurate extrapolation of the quantum defect into the positive energy region very difficult, the use of the QDM has been justly criticized.* At present, however, the QDM seems to be the best approximate procedure that exists for the calculation of photoionization cross sections for non-hydrogenic ions. The QDM is used here, and the results are examined for their sensitivity to the energy dependence of the quantum defect.

TABLE II. 4 gives the quantum defects for SI and SII. The wave numbers are from Moore (1949). Linear fits were obtained for the low \( n \) data points. The expressions, plotted in FIGURES II.1 and II.2 with the calculated quantum defects are:

\[
\begin{align*}
\text{SI}(^3S^0): \mu(\epsilon) &= 1.984 - 0.178\epsilon, \\
\text{SI}(^3D^0): \mu(\epsilon) &= 0.284 + 1.208\epsilon,
\end{align*}
\]  

(2.25)

*i.e. see Gould, et. al., Ap. J., 1967

-19-
\[
\text{SII}(^4\text{P}): \mu(\varepsilon) = 0.190 - 0.538\varepsilon, \\
\text{SII}(^2\text{P}): \mu(\varepsilon) = 1.504 - 0.121\varepsilon, \\
\text{SII}(^2\text{D}): \mu(\varepsilon) = -0.043 - 0.844\varepsilon, \\
\text{SII}(^2\text{F}): \mu(\varepsilon) = 0.160 - 0.609\varepsilon.
\]

(2.25)

In addition, to determine the sensitivity of resultant cross sections, expressions in Equations (2.25) were varied, and cross sections were also calculated using these values. The altered quantum defects were ones pertinent to photoionization from the ground states of SI and SII:

\[
\text{SI}(^3\text{S}^o): \quad \mu(\varepsilon) = 2.1 - 0.2\varepsilon, \\
\mu(\varepsilon) = 2.2 - 0.2\varepsilon, \\
\mu(\varepsilon) = 1.9 - 0.2\varepsilon, \\
\mu(\varepsilon) = 2.0 - 0.3\varepsilon, \\
\mu(\varepsilon) = 2.0 - 0.1\varepsilon.
\]

(2.26)

\[
\text{SI}(^3\text{D}^o): \quad \mu(\varepsilon) = 0.30 + 1.2\varepsilon, \\
\mu(\varepsilon) = 0.33 + 1.2\varepsilon, \\
\mu(\varepsilon) = 0.25 + 1.2\varepsilon, \\
\mu(\varepsilon) = 0.28 + 1.3\varepsilon, \\
\mu(\varepsilon) = 0.28 + 1.1\varepsilon.
\]

(2.27)

\[
\text{SII}(^4\text{P}): \quad \mu(\varepsilon) = 0.20 - 0.54\varepsilon, \\
\mu(\varepsilon) = 0.21 - 0.54\varepsilon, \\
\mu(\varepsilon) = 0.18 - 0.54\varepsilon, \\
\mu(\varepsilon) = 0.19 - 0.40\varepsilon, \\
\mu(\varepsilon) = 0.19 - 0.65\varepsilon.
\]

(2.28)
Further, the dependence of \( \mu \) upon the binding energy is demonstrated in FIGURE II.1, where an increase in the binding energy of 50 cm\(^{-1} \), or 0.00051 Ryd., lowers the calculated values of \( \mu(\varepsilon) \) for the \(^3D\) series to those indicated by the darkened squares (\( \mathcal{M} \)).
<table>
<thead>
<tr>
<th>Series</th>
<th>n</th>
<th>Energy (cm⁻¹)</th>
<th>μ (Rydbergs)</th>
</tr>
</thead>
<tbody>
<tr>
<td>SI(³S⁰)</td>
<td>4</td>
<td>55331.15</td>
<td>0.25723</td>
</tr>
<tr>
<td></td>
<td>5</td>
<td>71352.5</td>
<td>0.11124</td>
</tr>
<tr>
<td></td>
<td>6</td>
<td>76720.90</td>
<td>0.06232</td>
</tr>
<tr>
<td></td>
<td>7</td>
<td>79185.74</td>
<td>0.039850</td>
</tr>
<tr>
<td></td>
<td>8</td>
<td>80521.99</td>
<td>0.027675</td>
</tr>
<tr>
<td>SI(³D⁰)</td>
<td>3</td>
<td>70166.8</td>
<td>0.12204</td>
</tr>
<tr>
<td></td>
<td>4</td>
<td>75952.67</td>
<td>0.069311</td>
</tr>
<tr>
<td></td>
<td>5</td>
<td>78692.24</td>
<td>0.044351</td>
</tr>
<tr>
<td></td>
<td>6</td>
<td>80183.93</td>
<td>0.030755</td>
</tr>
<tr>
<td></td>
<td>7</td>
<td>81082.83</td>
<td>0.012563</td>
</tr>
<tr>
<td></td>
<td>8</td>
<td>81666.0</td>
<td>0.017250</td>
</tr>
<tr>
<td>SII(⁴P)</td>
<td>4</td>
<td>109831.28</td>
<td>0.71984</td>
</tr>
<tr>
<td></td>
<td>5</td>
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<td>0.34895</td>
</tr>
<tr>
<td>SII(²P)</td>
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<td>0.69154</td>
</tr>
<tr>
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<td>151910.67</td>
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</tr>
<tr>
<td>SII(²D)</td>
<td>3</td>
<td>119242.13</td>
<td>0.63408</td>
</tr>
<tr>
<td></td>
<td>4</td>
<td>158666.45</td>
<td>0.27482</td>
</tr>
<tr>
<td>SII(²F)</td>
<td>3</td>
<td>114804.11</td>
<td>0.67452</td>
</tr>
<tr>
<td></td>
<td>4</td>
<td>156121.33</td>
<td>0.29801</td>
</tr>
</tbody>
</table>
FIGURE II-1. The quantum defects of the $3S$ and $3D$ series of neutral sulphur. Linear fits are drawn to the lower (n), more accurate, values.

FIGURE II-2. The quantum defects of the $2P$, $2D$, $2F$ and $4P$ series of singly-ionized sulphur. Linear fits are drawn to the lower (n), more accurate, values.
FIGURE II.1

BINDING ENERGY (Ryd.)

$\mu^{(3S)}$

$\mu^{(3D)}$

$^3S$ QUANTUM DEFECT FOR SI

$^3D$ QUANTUM DEFECT FOR SI
2. The Quantum Defect Method

The cross section for photoionization of an atom (or ion), initially in state $|i\rangle$, is the probability of the ionization occurring, divided by the flux of incident photons. If there is one photon of energy $\hbar \omega$ in a given volume, in the dipole approximation the photoionization cross section can be written as

$$\alpha_{fi} = \frac{\pi e^2}{3\varepsilon_0 c} \sum_j |\langle f|x_j|i\rangle|^2$$

(2.29)

$|f\rangle$ is the final state - ion plus ejected electron, and the $x_j$ are Cartesian coordinates for the continuum electron. If there is more than one initial and/or final state of fixed energy, the summation in Equation (2.29) must also include all of them. Let $\omega_i$ be the degeneracy of the initial state. A quantity $S$ may be defined so that

$$\alpha_{fi} = \frac{4\pi \alpha a_0^2}{3} (\chi_i + Z^2 \varepsilon) \frac{S}{\omega_i}$$

(2.30)

where $\alpha$ is the fine structure constant, $a_0$ is the Bohr radius, and as before, $\hbar \omega = \chi_i + Z^2 \varepsilon$.

From Equations (2.29) and (2.30), it follows that

$$S = \Sigma^\dagger \Sigma |\langle f|\frac{x_i}{a_0^2}|i\rangle|^2$$

(2.31)

$\Sigma^\dagger$ denotes the additional sum mentioned above. If L-S coupling accurately describes the initial and final states,

*The reader wishing to refresh his memory on the general theory of photoionization is referred to Appendix B.*
and if the photo-ejected electron is represented by a wave function orthogonal to all bound state wave functions, Burgess and Seaton have shown

\[
\frac{S}{\omega} = \sum_{l'=l+1}^{\infty} \sum_{L'=L,L+1} C_{l',L'} \left| \int_0^\infty P_{nL}(r) G_{kL'}(r) \, rdr \right|^2 \tag{2.32}
\]

The \( C_{l',L'} \) are algebraic factors obtained from integrations over appropriate angular coordinates. \( P_{nL}(r) \) and \( \frac{1}{r} G_{kL'}(r) \) are the radial portions of the bound \((nL)\) electron's and ejected \((kL')\) electron's wave functions.

By the quantum defect approximation the radial integral in (2.32) can be calculated from

\[
\int_0^\infty P_{nL}(r) G_{kL'}(r) \, rdr = \frac{1}{\chi_{nL}} g(v'L;\varepsilon L') \tag{2.33}
\]

with

\[
\chi_{nL} = \text{binding energy (Ryd.) of the \((nL)\) electron}
\]

\[
g(v'L;\varepsilon L') = \frac{G(v'L;\varepsilon L')}{\zeta(v'L)} \cos \pi [v'\mu'(\varepsilon) + \chi(v'L;\varepsilon L')]
\]

\[
G(v'L;\varepsilon L') = (-1)^{l+1} G_{lL'}(v') \left[ 1 + \varepsilon(v')^2 \right]^{-\gamma L L'}(v')
\]

\[
\chi(v'L;\varepsilon L') = \chi_{lL'}(v') + \alpha_{lL'} \left[ \frac{\varepsilon v'}{1 + \varepsilon(v')} \right] + \beta_{lL'}(v') \left[ \frac{\varepsilon(v')^2}{1 + \varepsilon(v')^2} \right]
\]

\[
\zeta(v'L) = 1 + \frac{2}{(v')^3} \frac{a}{\delta \varepsilon} \mu(\varepsilon)
\]

\( \mu(\varepsilon) \) is the quantum defect of the \((nL)\) series; \( \mu'(\varepsilon) \) is the extrapolated quantum defect of the \((n'L')\) series. All of
the above parameters have been tabulated by Burgess and Seaton (1960). Graphs of the pertinent functions are given here, FIGURES II-3 and II-4, and values used in calculating cross sections are listed in TABLE II.5.

Summarizing, the photoionization cross section for an electron with binding energy $X_{nl}^\prime$ is given by the quantum defect method as

$$
\alpha = 8.559 \times 10^{-19} \left[ \frac{X_{nl} + Z^2 \epsilon}{X_{nl}^2} \right] \sum_{l',L'} |g(v'l';\epsilon')|^2 \text{ cm}^2 \tag{2.34}
$$

Equation (2.34) is used to calculate cross sections for the collisions indicated at the beginning of this discussion. The results are plotted in FIGURES II-5 - II-7. For comparison hydrogenic photoionization cross sections, proportional to $1/v^3$, are also shown. So far as the author knows, photoionization cross sections for neutral and singly ionized sulphur have neither been calculated nor measured previously.

FIGURES II-8 and II-9 are the cross sections obtained for different quantum defect energy dependences. It can be seen that these cross sections are not inordinately dependent upon the quantum defects used, at least as long as the general slope of $\mu(\epsilon)$ is retained.
FIGURES II-3, 4. The various parameters, given by Burgess and Seaton (1960) and used to calculate the photoionization cross sections of neutral and singly-ionized sulphur, are graphed. The values in FIGURE II-3(4) are to be used when the photo-ejected electron has an orbital angular momentum quantum number $l = 2(0)$. 
\[ np - k^2 d \]

PHOTOIONIZATION PARAMETERS

\[ \frac{G_{12}}{(\gamma' - 1)^{\frac{1}{2}}} \]

\[ G_{12} \]

\[ \gamma_{12} \]

\[ \theta_{12} \]

\[ \chi_{12} \]

FIGURE II-3
FIGURE II-4

PHOTOIONIZATION PARAMETERS

\( \eta \rightarrow k^2 \)
### TABLE II.5

SI AND SII PHOTOIONIZATION PARAMETERS (from Burgess and Seaton)

<p>| Z | Transition | $X_{n\ell}$ (Ryd) | $v'$ | $\ell'$ | Extrapolated Series | $C_{\ell'\ell}$ | $\gamma_{\ell\ell'}(v')$ | $X_{\ell\ell'}(v')$ | $G_{\ell\ell'}(v')$ | $\beta_{\ell\ell'}(v')$ |
|---|------------|-------------------|-----|--------|---------------------|---------------|----------------|----------------|-------------|----------------|---------------|
| 1 | $^3P \rightarrow ^4S^0$ | 0.761 | 1.15 | 0 | $^3S^0$ | 4/9 | 1.49 | -0.27 | 1.56 | 0 |
| 1 | $^3P \rightarrow ^4S^0$ | 0.761 | 1.15 | 2 | $^3D^0$ | 8/9 | 1.97 | 0.54 | 5.61 | 0.070 |
| 1 | $^3P \rightarrow ^2D^0$ | 0.761 | 1.15 | 0 | $^3D^0$ | 5/9 | 1.49 | -0.27 | 1.56 | 0 |
| 1 | $^3P \rightarrow ^2D^0$ | 0.761 | 1.15 | 2 | $^3S^0$ | 2/9 | 1.97 | 0.54 | 5.61 | 0.070 |
| 1 | $^3P \rightarrow ^2D^0$ | 0.761 | 1.15 | 2 | $^3D^0$ | 7/18 | 1.97 | 0.54 | 5.61 | 0.070 |
| 1 | $^3P \rightarrow ^2P^0$ | 0.761 | 1.15 | 2 | $^3D^0$ | 1/2 | 1.97 | 0.54 | 5.61 | 0.070 |
| 2 | $^4S^0 \rightarrow ^3P$ | 1.72 | 1.51 | 0 | $^4P$ | 1 | 1.62 | -0.25 | 1.23 | 0 |
| 2 | $^4S^0 \rightarrow ^3P$ | 1.72 | 1.51 | 2 | $^4P$ | 2 | 1.65 | 0.32 | 4.56 | 0.040 |
| 2 | $^2D^0 \rightarrow ^3P$ | 1.58 | 1.59 | 0 | $^2P$ | 1/2 | 1.63 | -0.25 | 1.18 | 0 |
| 2 | $^2D^0 \rightarrow ^3P$ | 1.58 | 1.59 | 2 | $^2P$ | 1/100 | 1.62 | 0.28 | 4.25 | 0.040 |
| 2 | $^2D^0 \rightarrow ^3P$ | 1.58 | 1.59 | 2 | $^2D$ | 3/20 | 1.62 | 0.28 | 4.25 | 0.040 |
| 2 | $^2D^0 \rightarrow ^3P$ | 1.58 | 1.59 | 2 | $^2F$ | 21/25 | 1.62 | 0.28 | 4.25 | 0.040 |</p>
<table>
<thead>
<tr>
<th>Z</th>
<th>Transition</th>
<th>$\chi_{n\ell}$ (Ryd)</th>
<th>$\nu'$</th>
<th>$\ell'$</th>
<th>Extrapolated Series</th>
<th>$C_{\ell'\prime L'}$</th>
<th>$\gamma_{\ell\ell'}(\nu')$</th>
<th>$\chi_{\ell\ell'}(\nu')$</th>
<th>$G_{\ell\ell'}(\nu')$</th>
<th>$\frac{(\nu'-1)\nu^2}{\beta_{\ell\ell'}(\nu')}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>2</td>
<td>$^2D^0 \rightarrow ^1D$</td>
<td>1.58</td>
<td>1.59</td>
<td>0</td>
<td>$^2D$</td>
<td>1/2</td>
<td>1.63</td>
<td>-0.25</td>
<td>1.18</td>
<td>0</td>
</tr>
<tr>
<td>2</td>
<td>$^2D^0 \rightarrow ^1D$</td>
<td>1.58</td>
<td>1.59</td>
<td>2</td>
<td>$^2P$</td>
<td>9/100</td>
<td>1.62</td>
<td>0.28</td>
<td>4.25</td>
<td>0.040</td>
</tr>
<tr>
<td>2</td>
<td>$^2D^0 \rightarrow ^1D$</td>
<td>1.58</td>
<td>1.59</td>
<td>2</td>
<td>$^2D$</td>
<td>7/20</td>
<td>1.62</td>
<td>0.28</td>
<td>4.25</td>
<td>0.040</td>
</tr>
<tr>
<td>2</td>
<td>$^2D^0 \rightarrow ^1D$</td>
<td>1.58</td>
<td>1.59</td>
<td>2</td>
<td>$^2F$</td>
<td>42/75</td>
<td>1.62</td>
<td>0.28</td>
<td>4.25</td>
<td>0.040</td>
</tr>
<tr>
<td>2</td>
<td>$^2P^0 \rightarrow ^3P$</td>
<td>1.49</td>
<td>1.64</td>
<td>0</td>
<td>$^2P$</td>
<td>1/2</td>
<td>1.64</td>
<td>-0.25</td>
<td>1.16</td>
<td>0</td>
</tr>
<tr>
<td>2</td>
<td>$^2P^0 \rightarrow ^3P$</td>
<td>1.49</td>
<td>1.64</td>
<td>2</td>
<td>$^2P$</td>
<td>1/4</td>
<td>1.61</td>
<td>0.26</td>
<td>4.15</td>
<td>0.025</td>
</tr>
<tr>
<td>2</td>
<td>$^2P^0 \rightarrow ^3P$</td>
<td>1.49</td>
<td>1.64</td>
<td>2</td>
<td>$^2D$</td>
<td>3/4</td>
<td>1.61</td>
<td>0.26</td>
<td>4.15</td>
<td>0.025</td>
</tr>
<tr>
<td>2</td>
<td>$^2P^0 \rightarrow ^1D$</td>
<td>1.49</td>
<td>1.64</td>
<td>0</td>
<td>$^2D$</td>
<td>5/18</td>
<td>1.64</td>
<td>-0.25</td>
<td>1.16</td>
<td>0</td>
</tr>
<tr>
<td>2</td>
<td>$^2P^0 \rightarrow ^1D$</td>
<td>1.49</td>
<td>1.64</td>
<td>2</td>
<td>$^2P$</td>
<td>1/4</td>
<td>1.61</td>
<td>0.26</td>
<td>4.15</td>
<td>0.025</td>
</tr>
<tr>
<td>2</td>
<td>$^2P^0 \rightarrow ^1D$</td>
<td>1.49</td>
<td>1.64</td>
<td>2</td>
<td>$^2D$</td>
<td>7/36</td>
<td>1.61</td>
<td>0.26</td>
<td>4.15</td>
<td>0.025</td>
</tr>
<tr>
<td>2</td>
<td>$^2P^0 \rightarrow ^1S$</td>
<td>1.49</td>
<td>1.64</td>
<td>2</td>
<td>$^2D$</td>
<td>4/9</td>
<td>1.61</td>
<td>0.26</td>
<td>4.15</td>
<td>0.025</td>
</tr>
</tbody>
</table>
In FIGURE II-9, the labeling refers to the following quantum defects (see Equation 2.28):

<table>
<thead>
<tr>
<th>( \mu[\text{II}(^4\text{P})] )</th>
<th>1</th>
<th>0.10 - 0.54( \text{e} )</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>2</td>
<td>0.20 - 0.54( \text{e} )</td>
</tr>
<tr>
<td></td>
<td>3</td>
<td>0.21 - 0.54( \text{e} )</td>
</tr>
</tbody>
</table>

The other quantum defects in Equation (2.28) did not alter the cross section noticeably.
FIGURES II-5,6,7. The photoionization cross sections of the ground state of neutral sulphur and the five states of the SII(3p$^3$) configuration. Calculations were performed using the QDM outlined by Burgess and Seaton (1960).

For comparison, a cross section proportional to $\nu^{-3}$ (hydrogenic) is also displayed.

FIGURES II-8,9. The changes in the photoionization cross sections, for the transitions SI($^3P$)$\rightarrow$SII($^4S$) and SII($^4S$)$\rightarrow$SIII($^3P$), to variations of the appropriate quantum defects.

In FIGURE II-8, the labeling refers to the following quantum defects (see Equations 2.26-27):

<table>
<thead>
<tr>
<th></th>
<th>$\mu$(SI($^3S^\circ$))</th>
<th>$\mu$(SI($^3D^\circ$))</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>$2.0 - 0.2\epsilon$</td>
<td>$0.28 + 1.2\epsilon$</td>
</tr>
<tr>
<td>2</td>
<td>$2.1 - 0.2\epsilon$</td>
<td>$0.30 + 1.2\epsilon$</td>
</tr>
<tr>
<td>3</td>
<td>$2.2 - 0.2\epsilon$</td>
<td>$0.33 + 1.2\epsilon$</td>
</tr>
<tr>
<td>4</td>
<td>$1.9 - 0.2\epsilon$</td>
<td>$0.25 + 1.2\epsilon$</td>
</tr>
<tr>
<td>5</td>
<td>$2.0 - 0.3\epsilon$</td>
<td>$0.28 + 1.3\epsilon$</td>
</tr>
<tr>
<td>6</td>
<td>$2.0 - 0.1\epsilon$</td>
<td>$0.28 + 1.1\epsilon$</td>
</tr>
</tbody>
</table>
SULPHUR I PHOTOIONIZATION CROSS SECTION

\[ \alpha \propto \gamma^3 \]

- [\text{Si}] \rightarrow [\text{SiI}]
- \text{3p} \rightarrow 4\text{S}
- \text{3p} \rightarrow 2\text{D}
- \text{3p} \rightarrow 2\text{p}

\( \alpha \times 10^3 \) cm²

ENERGY OF EJECTED ELECTRON (Ryd.)

\( 0.1 \quad 0.2 \quad 0.3 \quad 0.4 \quad 0.5 \quad 0.6 \)
FIGURE II-6
SULPHURII PHOTONIZATION CROSS SECTION

ENERGY OF EJECTED ELECTRON (Ry)

$\sigma \propto k^3$

FIGURE II-7
VARIATION OF PHOTOIONIZATION CROSS SECTION WITH RESPECT TO THE QUANTUM DEFECT

$SI(^3P) \rightarrow SII(^4S)$

FIGURE II-8
VARIATION OF PHOTOIONIZATION CROSS SECTION WITH RESPECT TO THE QUANTUM DEFECT

$\text{SII}^{(4S)} \rightarrow \text{SIII}^{(3P)}$

$\sigma \times 10^{-17} \text{cm}^2$

ENERGY OF EJECTED ELECTRON (Ryd.)
3. Results

The cross sections described above were used to calculate the related photoionization rates:

\[ \psi_{f1} = 9.94 \times 10^{26} N_i \bar{W} z^2 \int_{0}^{\infty} \frac{(\chi_i + Z^2 \varepsilon)^2 \alpha_{f1}(\varepsilon)}{\exp \left( \frac{\chi_i + Z^2 \varepsilon}{kT} \right) - 1} \, d\varepsilon. \]  

Equation (2.35) was integrated numerically over the range of temperatures: 5000°K < Te < 30000°K. TABLE II.6 displays the results in the form \( (\psi_{xy})^N \bar{W} = D_{xy} \), a function that can be considered an ionization rate coefficient. Levels of the same term are assumed to be populated according to their statistical weights.

Because the photoionization cross section for SII(4S) \( \rightarrow \) SIII(3P) is quite insensitive to small variations in \( \mu(\varepsilon) \), the ionization rate coefficient shows little change when any of Equations (2.28) are substituted. The sensitivity of the SI(3P) \( \rightarrow \) SII(4S) cross section to the quantum defect produces less than ten percent variations from the ionization rate coefficients given in TABLE II.6 for that transition.

Also it might be pointed out that integrating Equation (2.35) from \( \varepsilon = 0 \) to \( \varepsilon = 0.1 \) Ryd. yields approximately three-fourths of the total value of the integral. Since the Q.D.M. is usually valid only for small positive energies, errors introduced into the photoionization rates due to cross sections inaccurately known at energies \( \varepsilon > 0.1 \) Ryd. should be small.
TABLE II.6
PHOTOIONIZATION RATE COEFFICIENTS FOR SI AND SII

<table>
<thead>
<tr>
<th>INITIAL STATE</th>
<th>FINAL STATE</th>
<th>PHOTOIONIZATION RATE COEFFICIENT, D</th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>$T_e=5000^\circ K$</td>
<td>$T_e=10000^\circ K$</td>
<td>$T_e=15000^\circ K$</td>
</tr>
<tr>
<td>SI($^3P$)</td>
<td>SII($^4S$)</td>
<td>$2.03\times10^{-2}$</td>
<td>$8.58\times10^3$</td>
<td>$6.40\times10^5$</td>
</tr>
<tr>
<td>SI($^3P$)</td>
<td>SII($^2D$)</td>
<td>$1.10\times10^{-2}$</td>
<td>$4.76\times10^3$</td>
<td>$3.62\times10^5$</td>
</tr>
<tr>
<td>SI($^3P$)</td>
<td>SII($^2P$)</td>
<td>$1.10\times10^{-2}$</td>
<td>$4.65\times10^3$</td>
<td>$3.45\times10^5$</td>
</tr>
<tr>
<td>SII($^4S$)</td>
<td>SIII($^3P$)</td>
<td>$1.10\times10^{-2}$</td>
<td>$4.17\times10^{-2}$</td>
<td>$2.73\times10^2$</td>
</tr>
<tr>
<td>SII($^2D$)</td>
<td>SIII($^3P$)</td>
<td>$3.58\times10^{-2}$</td>
<td>$3.14\times10^2$</td>
<td>$1.69\times10^6$</td>
</tr>
<tr>
<td>SII($^2D$)</td>
<td>SIII($^1D$)</td>
<td>$1.02\times10^{-1}$</td>
<td>$4.10\times10^2$</td>
<td>$1.81\times10^6$</td>
</tr>
<tr>
<td>SII($^2P$)</td>
<td>SIII($^3P$)</td>
<td>$2.81\times10^{-2}$</td>
<td>$1.13\times10^2$</td>
<td>$4.96\times10^5$</td>
</tr>
<tr>
<td>SII($^2P$)</td>
<td>SIII($^1D$)</td>
<td>$5.55\times10^{-2}$</td>
<td>$2.23\times10^2$</td>
<td>$9.90\times10^5$</td>
</tr>
</tbody>
</table>
E. Collisional Ionization Rates of SI and SII

In addition to photoionizations, inelastic collisions of atoms with energetic electrons can also produce ionizations. A general theory of atomic and ionic ionization is discussed at length by Seaton (1962). In conformance with his results, the cross section for an atom-electron ionizing collision (ground state-ground state) can be expressed as

$$\sigma_{\text{ioniz}}(\text{cm}^2) = 1.63 \times 10^{-18} n \left( \frac{1}{\chi(\text{ev})} \right)^2 \left( \frac{\chi}{e} \right) F(Z, \varepsilon/\chi)$$  \hspace{1cm} (2.36)

$Z$ is the charge on the residual ion; $n$ is the number of optical (valence) electrons; $\chi$ is the ionization potential. $(\chi/e)F(Z, \varepsilon/\chi)$ is frequently referred to as the reduced cross section. Allen (1963), § 18, has tabulated experimentally determined values of $F(Z, \varepsilon/\chi)$ for $Z = 1$ and 2, and suggests an accuracy of ten percent may be expected.

Collision rates involve integrals of the form

$$\int \sigma(v) v f(v) dv$$

so simple analytic expressions for $F$ were fit to the data of Allen. The expressions obtained were

$$F(1, \varepsilon/\chi) = 1.1 \left( \frac{\varepsilon}{\chi} - 1 \right)$$  \hspace{1cm} (2.37a)

$$F(2, \varepsilon/\chi) = -0.15 \left( \frac{\varepsilon}{\chi} \right)^2 + 1.95 \left( \frac{\varepsilon}{\chi} \right) - 1.80$$  \hspace{1cm} (2.37b)

These two functions are plotted in FIGURES II-10, in addition to the Allen data.

With this information, the rate of collisional ionization of state X[X being SI(3P) or SII(4S)],
FIGURE 11-10. The points $F(Z; \epsilon/\chi)$ are plotted for $Z=1$ and 2. Quadratic fits to the data are also displayed.

The quantity

$$q = (\kappa/\epsilon)F(Z; \epsilon/\chi)$$

is called the reduced cross section.
FIGURE II-10

SEATON'S COLLISIONAL IONIZATION FACTOR

\[-0.15 \left( \frac{e}{\chi} \right)^2 + 1.95 \left( \frac{e}{\chi} \right) - 1.80\]

\[1.1 \left( \frac{e}{\chi} - 1 \right)\]

○ F(1; e/χ)

△ F(2; e/χ)
\[ M_x = \frac{N_e N_x}{N} \int_{\text{threshold}}^{\infty} \sigma_{\text{ioniz}} f(v) \, dv \]  

(2.38)

can be numerically calculated. The notation here is that of Equations (2.2) and (2.3). Again transforming to an integral over electron energy, \( \varepsilon \), using Rydberg units Equation (2.38) becomes

\[ M_{\text{SI}} = 7.17 \times 10^{-6} \frac{N_e N_{\text{SI}}}{T_e^{3/2}} \int_{\chi(\text{SI})}^{\infty} F(1, \varepsilon/X) e^{-\varepsilon/kT} d\varepsilon \]  

(2.39a)

\[ M_{\text{SII}} = 2.38 \times 10^{-6} \frac{N_e N_{\text{SII}}}{T_e^{3/2}} \int_{\chi(\text{SII})}^{\infty} F(2, \varepsilon/X) e^{-\varepsilon/kT} d\varepsilon \]  

(2.39b)

The integrals (2.39a) and (2.39b) were performed using the same electron temperatures as those used in the inelastic collision rate integrals. Similarly, collisional ionization rate coefficients, \( (M_x/N_e N_x)_x \), are given in TABLE II.7.

Since all of the five lowest states of SII have the same configuration, \( (3p^3) \), it is assumed that each state receives a fraction of \( M_I \) that is determined by its statistical weight:

\[ \frac{2}{3} M_I \] populates the quartet state \( ^4S_{3/2} \);

\[ \frac{1}{3} M_I \] populates the doublet states, with

\[ \frac{1}{8} \left( \frac{1}{3} M_I \right) \] populating \( ^2P_{1/2} \),

\[ \frac{1}{4} \left( \frac{1}{3} M_I \right) \] populating \( ^2P_{3/2} \),

\[ \frac{3}{8} \left( \frac{1}{3} M_I \right) \] populating \( ^2D_{5/2} \),

\[ \frac{1}{4} \left( \frac{1}{3} M_I \right) \] populating \( ^2D_{3/2} \).
The extensive literature on the physical processes in nebulae indicate that the preceding collisional events are those important in interpreting the spectra observed. The relevant radiative processes are discussed in the next section.
<table>
<thead>
<tr>
<th>Electron Temp. $T_e$ (°K)</th>
<th>SI Ionization Rate Coeff.</th>
<th>SII Ionization Rate Coeff.</th>
</tr>
</thead>
<tbody>
<tr>
<td>5,000</td>
<td>$6.36 \times 10^{-19}$</td>
<td>$9.49 \times 10^{-33}$</td>
</tr>
<tr>
<td>10,000</td>
<td>$2.34 \times 10^{-13}$</td>
<td>$1.34 \times 10^{-19}$</td>
</tr>
<tr>
<td>15,000</td>
<td>$1.66 \times 10^{-11}$</td>
<td>$1.48 \times 10^{-16}$</td>
</tr>
<tr>
<td>30,000</td>
<td>$1.31 \times 10^{-9}$</td>
<td>$1.81 \times 10^{-12}$</td>
</tr>
</tbody>
</table>
III. RADIATIVE PROCESSES

Herein, radiative processes are taken to be those in which the final state of an interaction is characterized by photon emission. The events considered are radiative recombination and de-excitation.

Recombination of an ion and an electron, with a photon being emitted to conserve energy and momentum, is the time-reversed process of photoionization, discussed earlier. In this section the relations between photoionization and recombination cross sections and rates are derived, and values for the recombination rates of interest are estimated.

The theory concerning probabilities for bound-bound transitions is not discussed here. Recent calculations of the appropriate Einstein transition probabilities (A values) by Czyzak and Krueger (1963) are listed for convenience. Their data are used in this thesis.
A. Radiative De-excitation Rates for SII (3p$^3$)

The rate at which an excited state of an atom (or ion) is depopulated by radiative emission is simply the product of the number density of atoms (ions) in the upper state, $N_x$, and the total probability, $P_x$, for transition to another state. In Equation (3.1), this probability is given as

$$P_x = \sum_y A_{xy} \text{(sec}^{-1}).$$

If one is concerned with the rate of a specific transition, $R_{xy}$, then there is only one term in the above expression so that

$$R_{xy} = N_x A_{xy} \text{(cm}^{-3}\text{sec}^{-1}).$$

If, however, there is more than one type of transition possible, such as electric quadrupole or magnetic multipole transitions, $A_{xy}$, must be taken as the total of all individual transition probabilities.

$$A_{xy} = \sum_{\text{magnetic}} A_{xy} + \sum_{\text{electric}} A_{xy}. \quad (3.3)$$

The possibility of what are referred to as "forbidden", i.e. non-electric dipole, transitions occurring can be understood by the following argument.

The general approach for calculating transition probabilities involves evaluation of matrix elements like those encountered in the photoionization process (see Appendix B,
or a text such as Heitler [1954]):

\[
\langle \text{final state} | (e^{-i\vec{K}\cdot\vec{r}})\vec{p}\cdot\vec{a} | \text{initial state} \rangle.
\]

The dipole approximation sets \( e^{-i\vec{K}\cdot\vec{r}} = 1 \), but further expansion of the exponential allows calculations of matrix elements for \(-i\vec{K}\cdot\vec{r}, (-i\vec{K}\cdot\vec{r})^2/2!, \) etc., between the initial and final states. The electric dipole matrix element,

\[
\langle \text{final state} | (1)\vec{p}\cdot\vec{a} | \text{initial state} \rangle
\]

when not zero, is much greater than other multipole terms. But if it is zero, as it is between initial and final states of identical parity, then multipole terms, though small, still permit the transition to occur.

All of the SII terms considered arise from the same configuration, so they all have the same parity. As a consequence, only forbidden transitions occur between \(^4S_{3/2}\), \(^2D_{3/2, 5/2}\) and \(^2P_{1/2, 3/2}\). The calculations of Czyzak and Krueger (1963) of electric quadrupole (E2) and magnetic dipole (M1) transition probabilities for SII are reproduced in TABLE III-1. These probabilities are non-zero, and are much larger than still higher order terms. From this, Equation (3.3) indicates

\[
A_{xy} = A_{xy}(M1) + A_{xy}(E2). \quad (3.4)
\]

The \( A_{xy} \) are also given in TABLE III-1, and are used in the solution of the SII rate equations.
### TABLE III-1
SII TRANSITION PROBABILITIES*

<table>
<thead>
<tr>
<th>Transition</th>
<th>Type</th>
<th>Wavelength (Å)</th>
<th>Probability</th>
<th>A (total)</th>
</tr>
</thead>
<tbody>
<tr>
<td>$^{2}P_{3/2} - ^{2}P_{3/2}$</td>
<td>M1</td>
<td>--</td>
<td>$1.02 \times 10^{-6}$</td>
<td>$1.02 \times 10^{-6}$</td>
</tr>
<tr>
<td></td>
<td>E2</td>
<td></td>
<td>$8.93 \times 10^{-16}$</td>
<td></td>
</tr>
<tr>
<td>$^{2}D_{5/2} - ^{2}D_{3/2}$</td>
<td>M1</td>
<td>--</td>
<td>$3.33 \times 10^{-7}$</td>
<td>$3.33 \times 10^{-7}$</td>
</tr>
<tr>
<td></td>
<td>E2</td>
<td></td>
<td>$1.51 \times 10^{-16}$</td>
<td></td>
</tr>
<tr>
<td>$^{2}P_{3/2} - ^{2}D_{3/2}$</td>
<td>M1</td>
<td>10287</td>
<td>$1.08 \times 10^{-1}$</td>
<td>$1.74 \times 10^{-1}$</td>
</tr>
<tr>
<td></td>
<td>E2</td>
<td></td>
<td>$6.65 \times 10^{-2}$</td>
<td></td>
</tr>
<tr>
<td>$^{2}P_{3/2} - ^{2}D_{5/2}$</td>
<td>M1</td>
<td>10321</td>
<td>$6.02 \times 10^{-2}$</td>
<td>$2.14 \times 10^{-1}$</td>
</tr>
<tr>
<td></td>
<td>E2</td>
<td></td>
<td>$1.54 \times 10^{-1}$</td>
<td></td>
</tr>
<tr>
<td>$^{2}P_{1/2} - ^{2}D_{5/1}$</td>
<td>M1</td>
<td>10373</td>
<td>0.0</td>
<td>$8.65 \times 10^{-2}$</td>
</tr>
<tr>
<td></td>
<td>E2</td>
<td></td>
<td>$8.65 \times 10^{-2}$</td>
<td></td>
</tr>
<tr>
<td>$^{2}P_{1/2} - ^{2}D_{3/2}$</td>
<td>M1</td>
<td>10339</td>
<td>$6.65 \times 10^{-2}$</td>
<td>$1.98 \times 10^{-1}$</td>
</tr>
<tr>
<td></td>
<td>E2</td>
<td></td>
<td>$1.31 \times 10^{-1}$</td>
<td></td>
</tr>
<tr>
<td>$^{2}P_{3/2} - ^{4}S_{3/2}$</td>
<td>M1</td>
<td>4068.5</td>
<td>$3.41 \times 10^{-1}$</td>
<td>$3.41 \times 10^{-1}$</td>
</tr>
<tr>
<td></td>
<td>E2</td>
<td></td>
<td>$1.30 \times 10^{-6}$</td>
<td></td>
</tr>
<tr>
<td>$^{2}P_{1/2} - ^{4}S_{3/2}$</td>
<td>M1</td>
<td>4076.5</td>
<td>$1.34 \times 10^{-1}$</td>
<td>$1.34 \times 10^{-1}$</td>
</tr>
<tr>
<td></td>
<td>E2</td>
<td></td>
<td>$1.38 \times 10^{-5}$</td>
<td></td>
</tr>
<tr>
<td>$^{2}D_{5/2} - ^{4}S_{3/2}$</td>
<td>M1</td>
<td>6717.3</td>
<td>$3.63 \times 10^{-5}$</td>
<td>$4.65 \times 10^{-4}$</td>
</tr>
<tr>
<td></td>
<td>E2</td>
<td></td>
<td>$4.29 \times 10^{-4}$</td>
<td></td>
</tr>
<tr>
<td>$^{2}D_{3/2} - ^{4}S_{3/2}$</td>
<td>M1</td>
<td>6731.5</td>
<td>$1.56 \times 10^{-3}$</td>
<td>$1.83 \times 10^{-3}$</td>
</tr>
<tr>
<td></td>
<td>E2</td>
<td></td>
<td>$2.74 \times 10^{-4}$</td>
<td></td>
</tr>
</tbody>
</table>

*from Czyzak and Krueger (1963)
B. Radiative Recombination of SIII and SII

The rate at which an atom in a state \((x)\) is photoionized to some state \((y)\) by a photon with a frequency in the interval \(v\) to \(v + dv\) is given by Equation (2.17) as

\[
\frac{d\psi_{xy}}{v} = N_x \frac{4\pi I_\nu \alpha_{xy}(v) dv}{hv}. \tag{3.5}
\]

The reverse process is a collisional one, wherein a free electron recombines with an ion, and a photon is emitted. The rate of this process is

\[
\frac{d\phi_{yx}}{v} = N_x N_e f(v) \sigma_{yx}(v) v dv. \tag{3.6}
\]

\(f(v)\) is the electrons' velocity distribution function (Maxwellian), and \(\sigma_{yx}(v)\) is the recombination cross section. This recombination can be likened to spontaneous emission, since photons need not be present for the process to occur.

Now in thermodynamic equilibrium at a temperature \(T\), detailed balancing requires the total rate of emission, spontaneous plus induced, to be equal to the total rate of absorption, \(d\psi_{xy}\). As Feynman (1965) so aptly shows, basic properties of photons allow one to obtain the equilibrium relation

\[
\left(\frac{\text{Rate of spontaneous emission}}{\text{Rate of absorption}}\right) = 1 - e^{-\frac{hv}{kT}}. \tag{3.7}
\]

for photons of frequency \(v\). Substitution of the appropriate expressions for \(f\) and \(I_\nu\), with \(hv = \chi + \frac{1}{2}mv^2\), obtains
\[ \frac{N_x N_y}{N_e N_y} = \frac{8\pi \hbar^3}{(e\hbar/kT - 1)c^2 \hbar \nu \sigma_{y\chi}^{4\pi \nu^3 \hbar \nu}} \int_0^\infty \alpha_{x\chi}(v)e^{mv^2/2kT} dv \cdot \left[ \frac{2\pi kT}{m} \right]^{3/2} \]  

(3.8)

If Equation (3.8) is compared to the Saha ionization equilibrium equation, it is evident that

\[ \sigma_{y\chi}(v) = \frac{\omega_x}{\omega_y \frac{m}{m \nu c}} \alpha_{x\chi}(v) \]  

(3.9)

This equality, referred to in the literature as the Milne relation, contains only atomic parameters, and so does not depend upon external conditions.

Substituting the result of Equation (3.9) into Equation (3.6), integration over all incident electron velocities results in

\[ \phi_{y\chi} = \int_0^\infty \left[ \frac{\omega_x}{\omega_y} \left( \frac{\chi_x + \frac{1}{2} m \nu^2}{m v c} \right) \right]^2 \frac{4 \pi \nu^2}{\frac{m}{2 kT e}} \left[ \frac{m}{2 kT e} \right]^{3/2} \alpha_{x\chi}(v) ve^{mv^2/2kT e} dv \]

or with \( \frac{1}{2} m \nu^2 = Z^2 e^2 \),

\[ \phi_{y\chi} = \frac{N_x N_y}{N_e N_y} \left( \frac{\omega_x}{\omega_y} \right) \left( \frac{1}{m kT} \right)^{3/2} \frac{2}{\sqrt{2\pi} c^2} \frac{2}{Z^2 e} \]  

(3.10)

\[ \int_0^\infty (\chi_x + Z^2 e)^2 \alpha_{x\chi}(\epsilon)e^{-Z^2 e/kT} d\epsilon \]

The units of Equation (3.10) are c.g.s. Changing to atomic units, with energies measured in Rydbergs, evaluation of the constants in the above equation gives

-33-
as the rate of recombination \([\text{cm}^{-3}\text{sec}^{-1}]\). In this form specific recombinations can be calculated directly, once the corresponding ionization cross sections are known. Unfortunately, the complete rate of populating a state by ionic recombinations involves electron captures onto highly excited states and subsequent radiative decay, as well as direct recombination. Detailed treatments of hydrogen and helium recombinations by, among others, Burgess and Seaton (1960b), and Seaton (1959), indicate that a substantial fraction of the total recombinations is into excited states. This ultimately results in significant contributions to the population rates of lower states. A precise analysis of the sulphur problem, then, would require knowledge of an infinity of ionization cross sections and radiative transition probabilities. The two sections below describe the approximations used to produce calculable expressions for the recombination rates of interest.
1. Sulphur II

As seen by the data of Section II, the ionization - and hence recombination - rates are much smaller than the inelastic rates, collisional or radiative. An excited SII metastable state, then, is more likely to return to the ground state than recombine with an electron. Therefore,

\[ \text{SII}^{(4S_{1/2})} + e^- \rightarrow \text{SI} + \gamma \]

is considered the only important SII recombination process; in addition, only the total recombination rate is needed. Allen (1964) suggests that for non-hydrogenic recombinations, coefficients \( G_{ij} = \phi_{ij} / N_i N_e \), can be approximated by

\[ G(\text{to ground}) = 1 \times 10^{-11} Z^2 T_e^{-1/2} \text{cm}^3 \text{sec}^{-1}, \]
\[ G(\text{to all states}) = 3 \times 10^{-10} Z^2 T_e^{-3/4} \text{cm}^3 \text{sec}^{-1}. \] (3.12)

\( Z \) is the charge on the upper ion. Then

\[ G(\text{to all states}) = 30 G(\text{to ground state}) / T(0K)^{1/4}. \] (3.13)

The utility of this expression is that the photoionization cross section for \( \text{SI}(^3P) \rightarrow \text{SII}(^{4S_{1/2}}) \) is calculated by the QDM in Section II, and thus the recombination coefficient \( G(\text{to ground}) \) is known.

By Equations (3.11) and (3.13) it is easy to see that the rate of depopulation of \( \text{SII}(^{4S_{1/2}}) \) due to recombinations can be written from this approximation as
\[
\phi(\psi_{3/2} \rightarrow \text{SI}) = N(\psi_{3/2}) N_e \frac{9}{4} (30)(2.06 \times 10^{11}) T_e^{-7/4}.
\]

\[
\int \left( x_{\text{SII}} + \varepsilon \right)^2 \alpha(\psi_{3/2} \rightarrow 3p^0) e^{-\varepsilon/kT_e} d\varepsilon. \quad (3.14)
\]

From cross sections obtained in Section II, $\phi$ is calculated for the usual range of temperatures, and the recombination coefficients $G(\psi_{3/2}) = \phi(\psi_{3/2} \rightarrow 3p^0)/N(\psi_{3/2}) N_e$ and $G(\text{total})$ are listed in TABLE III.2.
2. Sulphur III

The photoionization cross sections obtained in Section II for the five denumerated states of singly-ionized sulphur enable the rates of recombination to these states to be calculated directly from Equation (3.11). Additional recombination occurs into the upper states of SII, with subsequent radiative decay into the five states specified. If this rate into upper states is denoted $\Phi_u = N(\text{SIII})N_e G_u$, a first approximation is to assume $2/3\Phi_u$ populates quartet states and $1/3\Phi_u$ populates doublet states, and, in addition, to assume that each of the four metastable doublet levels is ultimately populated by a fraction of the $1/3\Phi_u$ that is determined by its statistical weight, eg.

\[
\begin{align*}
\frac{2}{3}\Phi_u & \text{ populates } ^4S_{3/2} \\
\frac{1}{4} \times \frac{1}{3}\Phi_u & \text{ populates } ^2D_{3/2} \\
\frac{3}{8} \times \frac{1}{3}\Phi_u & \text{ populates } ^2D_{5/2} \\
\frac{1}{8} \times \frac{1}{3}\Phi_u & \text{ populates } ^2P_{1/2} \\
\frac{1}{4} \times \frac{1}{3}\Phi_u & \text{ populates } ^2P_{3/2}
\end{align*}
\]

The HeII recombination data obtained by Burgess and Seaton (1960) supports such a partitioning scheme. In fact, at $10,000 \ (20,000) \, ^oK$,

0.77 (0.78)$\Phi_u$ populates upper helium triplets,

0.23 (0.22)$\Phi_u$ populates upper helium singlets.
The ground state configurations for hydrogen (1s) and helium (1s\(^2\)) each give rise to a single term. SII(3p\(^3\)) however, yields three terms: \(^2P\), \(^2D\), \(^4S\). Since hydrogen and helium recombination coefficients are strongly dependent upon the principal quantum number of the recombining electron (\(G \propto \frac{1}{n^5}\) for hydrogen), the SII ground state recombination coefficient is taken as

\[
G(\text{to ground}) = G(\text{to } ^4S) + G(\text{to } ^2D) + G(\text{to } ^2P). \quad (3.16)
\]

The large separation between these terms and the terms with \(n > 4\) also suggests this approximation: indeed, the three coefficients are fairly equal - a fact borne out by data given in TABLE III.3.

The above expression determines \(\phi_u\):

\[
\phi_u = \phi_{\text{tot}} - \phi(\text{to ground}) = N_e N(\text{SIII}) G_u
\]

\[
= N_e N(\text{SIII}) \left[ 30T_e^{-\frac{1}{n}} - 1 \right] G(\text{to ground})
\]

\[
= N_e N(\text{SIII}) \left[ 30T_e^{-\frac{1}{n}} - 1 \right] \left[ G(\text{to } ^4S) + G(\text{to } ^2D) + G(\text{to } ^2P) \right] . \quad (3.17)
\]

Equation (3.17) is used to calculate the necessary recombination rate coefficients, the values of which are also given in TABLE III.3.

The recombination rate to a given term is assumed to populate levels of that term according to their statistical weights.
The accuracy of these data is difficult to determine, but comparison with the information on hydrogen and helium recombination (Seaton, 1959; Burgess and Seaton, 1960b) indicates that the values in TABLE III.3 should be correct to within an order of magnitude. The topics discussed in these last two chapters are needed to solve equations relating to the population rates of states of singly-ionized sulphur. In the next section the concept of abundance equilibrium is introduced and used to obtain the appropriate rate equations.
<table>
<thead>
<tr>
<th>Recombination Rate Coefficients</th>
<th>Electron Temperature (°K) x 10^{-4}</th>
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</thead>
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<tr>
<td>(10^{13} G(4S_{3/2} \rightarrow 3P_{\text{g}}))</td>
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</tr>
<tr>
<td>(10^{13} G_{\text{SII}}(\text{total}))</td>
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<td>(10^{13} G(\text{to } 2D))</td>
<td>4.86</td>
</tr>
<tr>
<td>(10^{13} G(\text{to } 2P))</td>
<td>1.78</td>
</tr>
<tr>
<td>(10^{13} G_u)</td>
<td>29.8</td>
</tr>
</tbody>
</table>
IV. ABUNDANCE EQUILIBRIUM OF SINGLY-IONIZED SULPHUR

As emphasized throughout preceding sections, the radiative and collisional processes that occur in gaseous nebulae tend to produce non-thermodynamic equilibrium distributions among atomic states. Apart from a general expansion of the nebular envelopes, however, observational data suggest that many steady-state conditions do exist. Prominent among these is the temporal constancy of nebular spectral intensities. By definition, the intensity $I$ of a line $\lambda$ is given by

$$I = N \frac{A h c}{\lambda} . \quad (4.1)$$

$N$ is the number density of ions in the upper state; $A$ is the probability for the transition of interest; $h c / \lambda$ is the energy of the emitted photon. It is evident from Equation (4.1) that a constant intensity implies a constant number density, $N$. And if $N$ does not change with time, the rate of populating the state is equal to its rate of depopulation:

$$\text{Rate in} = \text{Rate out} . \quad (4.2)$$

The rate equation (4.2) is a simple expression of the condition of abundance equilibrium.

The analysis of Sections II and III allow rate equations to be written for each of the states $^{2}P_{3/2},^{1/2}$, $^{2}D_{5/2},^{3/2}$, and $^{4}S_{3/2}$ of SII. To simplify notation these states will be
labeled 1, 2, ..., 5; in order of increasing energy: \(^4S_{3/2} \rightarrow 1, \quad ^2D_{3/2} \rightarrow 2, \) etc. Also, the ground states of \(\text{SI} \) and \(\text{SIII} \) are designated \(\text{I}, \) and \(\text{III}, \) respectively. Since all terms in the equations are in units \(\text{cm}^{-3} \text{sec}^{-1}, \) dimensions will not be noted explicitly. Symbols used below have been introduced earlier, but are given here for convenience.

\[
\begin{align*}
N_{\text{e}ab} & : \text{rate of recombination from (a) to (b)}; \\
N_{\text{a}eab} & : \text{rate of collisional excitation from (a) to (b)}; \\
N_{\text{a}}(\lambda) & : \text{rate of radiative decay of (a) due to emission of photon with wavelength } \lambda; \\
N_{\text{a}e} & : \text{rate of collisional ionization of (a)}; \\
N_{\text{a}WD} & : \text{rate of photoionization from (a) to (b)}.
\end{align*}
\]

Summations are over that part of the 5 low-lying states of \(\text{SII} \) indicated.

(1) Equilibrium Abundance of \(\text{SII}(^4S_{3/2}) \): Equation (4.3)

\[
\begin{align*}
N_e & N_{\text{III}} \left[\frac{2}{3} G_u + G_{\text{III},1} \right] + N_2 [N_e R_{21} + A(\lambda 6731)] \\
& + N_3 [N_e R_{31} + A(\lambda 6717)] + N_4 [N_e R_{41} + A(\lambda 4076)] \\
& + N_5 [N_e R_{51} + A(\lambda 4068)] + N_I [N_e \frac{2}{3} B_1 + \bar{WD}_{1,1}] = \\
& N_1 N_e \left[ \sum_{j=1}^{4} R_{1j} + B_1 + G_1 (\text{total}) \right] + N_1 \bar{WD}_{1,\text{III}}
\end{align*}
\]
(2) Equilibrium Abundance of SII($^{2}D_{3/2}$): Equation (4.4)

\[
N_{e}N_{III}\left[\frac{1}{12}G_{u} + G_{III,2}\right] + N_{1}N_{e}R_{12} + N_{3}\left[N_{e}R_{32} + A(3\rightarrow2)\right] + N_{4}\left[N_{e}R_{42} + A(\lambda 10339)\right] + N_{5}\left[N_{e}R_{52} + A(\lambda 10287)\right] + N_{I}\left[N_{e}\frac{1}{12}B_{I} + \bar{W}_{D_I,2}\right]
\]

\[
= N_{2}N_{e}\sum_{j\neq2} R_{2j} + N_{2}A(\lambda 6731)
\]

(3) Equilibrium Abundance of SII($^{2}D_{5/2}$): Equation (4.5)

\[
N_{e}N_{III}\left[\frac{1}{8}G_{u} + G_{III,3}\right] + N_{1}N_{e}R_{13} + N_{2}N_{e}R_{23}
\]

\[
+ N_{4}\left[N_{e}R_{43} + A(\lambda 10373)\right] + N_{5}\left[N_{e}R_{53} + A(\lambda 10321)\right]
\]

\[
+ N_{I}\left[N_{e}\frac{1}{8}B_{I} + \bar{W}_{D_I,3}\right]
\]

\[
= N_{3}N_{e}\sum_{j\neq3} R_{3j} + N_{3}[A(3\rightarrow2) + A(\lambda 6717)]
\]

(4) Equilibrium Abundance of SII($^{2}P_{3/2}$): Equation (4.6)

\[
N_{e}N_{III}\left[\frac{1}{24}G_{u} + G_{III,4}\right] + N_{e}\sum_{j=1}^{3} N_{j}R_{j,4}
\]

\[
+ N_{5}\left[N_{e}R_{54} + A(5\rightarrow4)\right] + N_{I}\left[N_{e}\frac{1}{24}B_{I} + \bar{W}_{D_I,4}\right]
\]

\[
= N_{4}N_{e}\sum_{j\neq4} R_{4j} + N_{4}[A(\lambda 4068) + A(\lambda 10339) + A(\lambda 10373)]
\]
(5) Equilibrium Abundance of SII($^{2}P_{3/2}$): Equation (4.7)

\[ N_e \frac{1}{12} G_u + G_{III,5} + N_e \sum_{j=1}^{4} R_{j5} N_j \]

\[ + N_I \left[ N_e \frac{1}{12} B_I + W_{I,5} \right] \]

\[ = N_{5} N_e \sum_{j \neq 5} R_{5j} + N_{5} [ A(\lambda 4076) + A(\lambda 10287) \]

\[ + A(\lambda 10321) + A(5-4) ] \]

Because they contribute negligibly, photoionization rates are not included in Equations (4.4) - (4.7) as a means of depopulating the excited states of SII.

Given an electron temperature $T_e$ and an electron number density $N_e$, the preceding five equations still involve seven unknown parameters - the number densities of the denumerated sulphur states. But useful studies in abundance equilibrium may be expressed in terms of relative number densities, $N_x/N(\text{reference state})$, so that only one additional relation between number densities of two or more states is needed to determine abundance equilibria in singly-ionized sulphur. Such a relation can be obtained from the ionization equilibrium that exists: there is a constant number of sulphur atoms in any given stage of ionization. Accordingly, the total ionization rate of neutral sulphur equals the total recombination rate of singly-ionized sulphur. In the notation used above,
Equations (4.3) - (4.8) were solved simultaneously for $N_i/N_1$ on the Rice University IBM 7040 computer. Electron temperatures used were $T_e = 5, 10, 15,$ and $30 \times 10^3 \text{°K}$. The electron number density was given values $N_e = 0.5, 0.75, 1.0, 2.5, 5.0, 7.5, 10,$ and $25 \times 10^3, 10^5, 10^6, 10^7, 10^9 \text{ cm}^{-3}$.

In addition, for every combination of $N_e$ and $T_e$ values, the rate equations were solved using the three values of the geometrical dilution factor, $\tilde{W} = 1, 5, \text{and } 10 \times 10^{-15}$. The solutions, however, were found to be insensitive to $\tilde{W}$: number density ratios $N_i/N_1$ varied by less than 1/10 of 1% as the dilution factor increased from 1 to $10 \times 10^{-15}$.

FIGURES (IV-1) - (IV-4) display the number density ratios $N(^2D_{3/2})/N(^4S_{3/2})$, $N(^2D_{5/2})/N(^4S_{5/2})$, $N(^2P_{1/2})/N(^4S_{3/2})$, and $N(^2P_{3/2})/N(^4S_{3/2})$ as functions of $N_e$, for each of the electron temperatures cited above. As expected at small values of the electron number density, the collisional population rates of these states are small, and radiative decays quickly return most of the excited ions to the ground state. As the number of electrons increases, the collision rates (proportional to $N_e$) also go up, producing a greater number of excited ions. Finally, the preponderance of electrons becomes so great ($10^9 \text{ cm}^{-3}$) that collisions completely dominate population rates and the number density ratios approach their thermodynamic equilibrium (Boltzmann) values.

Of greater applicability are the ratios $N(^2D_{5/2})/N(^2D_{3/2})$
FIGURES IV-1,2,3,4. The populations of the first four excited states of SII, relative to the ground state population, are presented as functions of electron number density for various electron temperatures.

In all cases the number density ratios first increase rapidly with electron density, and then asymptotically approach the Boltzmann (thermodynamic equilibrium) values for large electron number densities ($N_e \sim 10^9$ cm$^{-3}$).
Figure IV-1

Relative population of SII ($^2D_{3/2}$):

$$\frac{N(^2D_{3/2})}{N(^4S_{3/2})}$$

Log$_{10}$ electron number density (cm$^{-3}$)
RELATIVE POPULATION OF $S_{II}^2(^2D_{5/2})$:

$$\frac{N(^2D_{5/2})}{N(^2S_{3/2})}$$
RELATIVE POPULATION
OF \text{S} \text{II}(^{2}P_{\text{y}2}): \frac{N(^{2}P_{\text{y}2})}{N(^{4}S_{3/2})}

\log_{10} \text{ELECTRON NUMBER DENSITY (cm}^{3})

FIGURE IV-3
RELATIVE POPULATION OF SII\(^{2p_{3/2}}\):
\[ \frac{N^{(2p_{3/2})}}{N^{(4S_{3/2})}} \]

\( \log_{10} \) ELECTRON NUMBER DENSITY (cm\(^{-3}\))

FIGURE IV-4
and $N(\text{^2P}_{3/2})/N(\text{^2P}_{1/2})$; these are directly related to the intensity ratios of $\lambda 6717/\lambda 6731$ and $\lambda 4068/\lambda 4076$, respectively. Because of the relatively large (see TABLE III.1) transition probabilities of $\lambda 4068$ and $\lambda 4076$, and of the infrared lines $\lambda 10287$, $\lambda 10321$, $\lambda 10339$, and $\lambda 10373$, the ratio of ions in the $^2P$ states remained between 1.22 and 1.24 for $N_e \leq 10^5$ cm$^{-3}$, rising to its Boltzmann value (2.0) only after the electron number density was increased by several orders of magnitude. The intensity ratio of $\lambda 4068/\lambda 4076$, consequently was confined between 3.12 and 3.16 when $N_e \leq 10^5$ cm$^{-3}$.

On the other hand, the ratio of ions in the $^2D$ states was found to be quite sensitive to the electron density when $N_e \leq 10^5$ cm$^{-3}$, and somewhat dependent upon $T_e$. This is indicated by FIGURE IV.5, where $N(\text{^2D}_{5/2})/N(\text{^2D}_{3/2})$, i.e. $N_3/N_2$, is plotted as a function of $N_e$ for various electron temperatures. The corresponding intensity ratio of $\lambda 6717/\lambda 6731$ is also displayed.

Typical sensitivity of the $^2D$ ratio to the collision strengths is shown in FIGURE (IV.6), in which all $\Omega$'s were increased and decreased by 25%. The motivation for such an analysis was given by Seaton (1958), who noted that the relative accuracy of his collision strength calculations for OII was probably high, but the absolute accuracy might be off by as much as 40%. Further, because of the approximations made in Section II, a singular uncertainty exists.
with regards to the $\Omega(2\,^2D_{3/2},\,2\,^2D_{5/2})$ collision strength.* Accordingly, all other collision strengths were held at the values given in TABLE II.1, while $\Omega(2,3)$ was increased and decreased by 25%. The resulting solutions of the rate equations yield the $^2D$ density ratios given in FIGURE (IV.6) also.

In FIGURE (IV.7) results of present calculations, at $T_e = 10^4\,\text{K}$, are compared with the data of Naqvi and Talwar (1958), the only other specific analysis made of SII equilibrium abundances. Most of the difference is due to the fact that $\Omega(2,3)$, unknown at the time of their publication, was not included in the rate equations; also, improved values of the radiative transition probabilities have since become available.

The relative importance of various mechanisms in the population of the $^2D$ states is seen by the data in TABLE IV.1. Given are the percent contributions to the population rates of these two states, as functions of $N_e$ and $T_e$. The data show the following trend: for a given electron temperature, as $N_e$ becomes larger the contributions from the other excited states increase - a direct consequence of the fact that there are more inelastic collisions at larger $N_e$, and hence, more ions in the excited states. In thermodynamic equilibrium ($N_e = 10^9$), radiative processes are negligible.

*This statement also applies to $\Omega(2\,^2P_{1/2},\,2\,^2P_{3/2})$, but the collisional transition rate between the $^2P$ states is negligible in comparison to radiative decay rates from these two states.
FIGURE IV-5. The number density ratio 
\[ \frac{N(^2D_{5/2})}{N(^2D_{3/2})} \] is plotted as a function of electron number density for four values of the electron temperature. Also given is the corresponding intensity ratio for the transitions from the \(^2D\) states to the ground state.

FIGURE IV-6. The sensitivity of the \(^2D\) number density ratio to variations of collision strengths is indicated. The solid line is the same as that given in FIGURE IV-5 for an electron temperature of 10,000°K. The upper (lower) dashed curve indicates the ratio \[ \frac{N(^2D_{5/2})}{N(^2D_{3/2})} \] when \( \Omega (2,3) \) is increased (decreased) by 25%. The upper (lower) limits of the bars demonstrates the change in the \(^2D\) ratio when all collision strengths are increased (decreased) by 25%.

FIGURE IV-7. The values of \[ \frac{N(^2D_{5/2})}{N(^2D_{3/2})} \] obtained in this paper (at a temperature of 10^4°K) are compared to those obtained by an earlier analysis of Naqui and Talwar (1958).
NUMBER DENSITY RATIO OF \( \text{SII}(3p^2D) \) METASTABLE STATES

ELECTRON NUMBER DENSITY \( \text{(cm}^{-3} \text{)} \)

FIGURE IV-5
FIGURE IV-6

Sensitivity of the 
\[ \frac{N(^2D_{5/2})}{N(^2D_{3/2})} \]
SII \( (3p^2D) \) number density ratio to variation of the collision strengths

\[ T_e = 10,000 \, ^\circ \text{K} \]

Electron number density \( (\text{cm}^{-3}) \)
and collisional ionization of neutral sulphur accounts for most of the population rate not listed in the table.

The above data represent the more important information obtained from the solution of the SII rate equations. In the next section the applicability of these data to studies of gaseous nebulae is discussed.
NOTES ON TABLE IV.1

RCS2: population rate of state 2 ($^2D_{3/2}$) due to collisional excitation from state 1 ($^4S_{3/2}$).

RCD2: population rate of state 2 ($^2D_{3/2}$) due to collisional de-excitation from state 3 ($^2D_{5/2}$).

RRP2: population rate of state 2 ($^2D_{3/2}$) due to radiative decay from states 4 ($^2P_{3/2}$) and 5 ($^2P_{3/2}$).

RCS3: population rate of state 3 ($^2D_{5/2}$) due to collisional excitation from state 1 ($^4S_{3/2}$).

RCD3: population rate of state 3 ($^2D_{5/2}$) due to collisional excitation from state 2 ($^2D_{3/2}$).

RRP3: population rate of state 3 ($^2D_{5/2}$) due to radiative decay from states 4 ($^2P_{1/2}$) and 5 ($^2P_{3/2}$).
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<th>$N_e$ (cm$^{-3}$)</th>
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<th>5000</th>
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V. PROPERTIES OF GASEOUS NEBULAE

It has been fairly well established [Mathews (1966), Osterbrock (1964)] that the envelope of a planetary nebula is some admixture of material ejected from the central star and interstellar matter. Consequently, spectral information relating to the chemical composition and physical properties of nebulae can be applied to gain a better understanding of them - the processes of formation and maintenance, and the role of nebulae in stellar evolution.

For reference some of the observational data of planetary nebulae, collected over the last thirty years, is given in this section. The results of the preceding sections on the abundance equilibrium of singly-ionized sulphur is then used in conjunction with this information to estimate values of the electron number density in the regions of SII emission. The $N_e$ values are compared to those obtained by other techniques.

Finally, additional applications of the SII data are mentioned.
A. **Spectra and Composition**

Nebular envelopes, irradiated by the stars which they surround, display a great number of spectral lines. A comprehensive survey by Wyse (1942) of several nebulae revealed that almost forty percent of the lines were of unknown origin; since then, however, most of the lines have been identified. More recently Aller and his co-workers have obtained spectra for many nebulae. Their work, and that of Wyse, is partially summarized in TABLE V.1, which lists ions detected in eight nebular spectra. As seen from the table, most elements identified are present in more than one stage of ionization. This, together with the absence of thermodynamic equilibrium, makes chemical abundance determinations quite difficult. Estimated abundances (on the relative scale Oxygen = 1x10^8) for the nebulae listed in TABLE V.1 are given in TABLE V.2. In TABLE V.3, averages of the above abundance values are compared to those for other celestial objects. Note the similarities among the sun (a G2 star), B stars, and nebular envelopes.
NOTES ON TABLE V.1

1.Observers:

NGC 7027: Aller, Bowen and Minkowski (1955)
NGC 7662: Aller, Kaler, and Bowen (1966)
NGC 7009: Aller, Kaler (1964a)
IC 418: Aller, Kaler (1964b)
NGC 1976: Kaler, Aller, and Bowen (1965)
VV 267: Aller and Walker (1965)
NGC 6741: Aller and Walker (1965)
Wyse (1942)
NGC 6572: Wyse (1942)

2. Hydrogen and helium are not listed since all nebulae exhibit numerous lines of these two elements.

3. In addition to those listed, the following ions have been observed:

NGC 7027 - (Co V)::*
(O V)::*

NGC 7662 - (Na IV)::*
TABLE V.1
IONS OBSERVED IN THE SPECTRA OF 8 NEBULAE

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<th>NGC 7037</th>
<th>NGC 7662</th>
<th>NGC 7009</th>
<th>IC 418</th>
<th>#NGC 1976</th>
<th>VV 267</th>
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x: observed in 3200Å - 5000Å region
*: observed only in 5000Å - 7500Å region
?: questionable detection
#: Orion, NGC 1976, is a diffuse nebulae
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</table>
NOTES ON TABLE V.2

1. All abundances have been normalized to $O = 1 \times 10^4$ = relative number of oxygen atoms.

2. Blank spaces indicate spectral intensities were too uncertain to allow abundance determinations.

3. The abundances of metals are difficult to determine because inelastic cross sections are not well-known.

4. Sources:
   - NGC 7027: Aller (1954)
   - NGC 7662: Aller (1957)
   - NGC 7009: Aller (1961); Aller and Menzel (1945)
   - IC 418: Aller and Menzel (1945)
   - VV 267: Aller (1957)
   - NGC 6741: Aller (1957)
   - NGC 6572: Aller and Menzel (1945)
### TABLE V.2

CHEMICAL ABUNDANCES OF 8 NEBULAE

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</table>
### TABLE V.3
CHEMICAL COMPOSITIONS OF VARIOUS CELESTIAL OBJECTS

<table>
<thead>
<tr>
<th></th>
<th>Sun</th>
<th>B Stars</th>
<th>Nebulae</th>
<th>Novae</th>
</tr>
</thead>
<tbody>
<tr>
<td>H</td>
<td>1.1x10^7</td>
<td>1.7x10^7</td>
<td>3.1x10^7</td>
<td>2.3x10^6</td>
</tr>
<tr>
<td>He</td>
<td>1.8x10^6</td>
<td>2.7x10^6</td>
<td>3.6x10^6</td>
<td>3.7x10^5</td>
</tr>
<tr>
<td>C</td>
<td>5.7x10^3</td>
<td>3.3x10^3</td>
<td>1.0x10^4</td>
<td>7.6x10^2</td>
</tr>
<tr>
<td>N</td>
<td>1.1x10^6</td>
<td>2.6x10^3</td>
<td>5.6x10^3</td>
<td>1.2x10^4</td>
</tr>
<tr>
<td>O</td>
<td>1.0x10^6</td>
<td>1.0x10^4</td>
<td>1.0x10^4</td>
<td>1.0x10^4</td>
</tr>
<tr>
<td>Ne</td>
<td>5.5x10^3</td>
<td>8.8x10^3</td>
<td>2.4x10^3</td>
<td>6.4x10^2</td>
</tr>
<tr>
<td>Mg</td>
<td>2.8x10^2</td>
<td>1.5x10^3</td>
<td>---</td>
<td>---</td>
</tr>
<tr>
<td>Si</td>
<td>3.5x10^2</td>
<td>4.7x10^2</td>
<td>---</td>
<td>---</td>
</tr>
<tr>
<td>S</td>
<td>2.2x10^2</td>
<td>5.1x10^2</td>
<td>1.2x10^3</td>
<td>2.8x10^2</td>
</tr>
<tr>
<td>Cl</td>
<td>---</td>
<td>2.7x10</td>
<td>6.5x10</td>
<td>---</td>
</tr>
<tr>
<td>Ar</td>
<td>---</td>
<td>1.4x10^2</td>
<td>1.3x10^3</td>
<td>---</td>
</tr>
</tbody>
</table>

### NOTES ON TABLE V.3

1. The values under the entry "nebulae" are averages of the values in TABLE V.2 excluding NGC 1976, and refer to the envelopes only.

2. The "B star" values are an average (Aller, 1961) of numerous observations by several astronomers.

3. The Solar values are from Goldberg, Muller and Aller (1960), and Aller (1961).

4. The "novae" averages were collected by Pattasch (1958).
B. **Electron Densities and Temperatures**

The insensitivity of the ratio \( N(\text{D}_5/\text{D}_3) / N(\text{D}_5/\text{D}_3) \) to the electron temperature, demonstrated in FIGURE (IV.5), prevents estimates of \( T_e \) from being obtained from SII data. However, given a value for \( T_e \), electron number densities can be estimated. For simplicity, the electron temperatures adopted by Delmer, Gould, and Ramsey (1967) are used whenever possible. TABLE V.4 presents electron number densities estimated from the intensity ratio \( \lambda 6717/\lambda 6731 \). Values of \( N_e \) obtained by other techniques are given for comparison. The intensity ratios \( \lambda 6717/\lambda 6731 \) and \( \lambda 4068/\lambda 4076 \) are also listed.

Agreement among the various values of \( N_e \) is fairly good, except for IC 418 and NGC 6543. The disagreements may be due to the fact that the intensity ratio \( \lambda 6717/\lambda 6731 \) was available only in the pioneering work of Wyse (1942), and may be inaccurate.

It should also be pointed out that, as indicated by the data of the preceding section, the intensity ratio \( \lambda 4068/\lambda 4076 \) is insensitive to both \( N_e \) and \( T_e \) for typical nebular values. The solution of the rate equations gives an approximately constant ratio \( \lambda 4068/\lambda 4076 = 3.15 \). The observational data, though, consistently indicates a lower value. Such a discrepancy suggests that the relevant transition probabilities may be in error.
NOTES ON TABLE V.4

1. All temperatures are those adopted by Delmer, Gould, and Ramsey (1967), except for Orion [O'Dell (1966)].

2. Sources of data:
   a) Wyse (1942)
   b) Aller, Bowen and Minkowski (1955)
   c) Aller, Kaler, and Bowen (1966)
   d) Aller and Kaler (1964)
   e) Kaler, Aller and Bowen (1965)
   f) Swings and Jose (1949)
   g) Aller and Minkowski (1946)
   h) Delmer, Gould and Ramsey (1967)
   i) Aller (1956)
   j) O'Dell (1965)


<table>
<thead>
<tr>
<th>NEBULA</th>
<th>$T_e$ ($10^4 \text{K}$)</th>
<th>$\lambda 4068/\lambda 4076$</th>
<th>$\lambda 6717/\lambda 6731$</th>
<th>$N_e$ ($10^4 \text{cm}^{-3}$) (this paper)</th>
<th>$N_e$ ($10^4 \text{cm}^{-3}$) (other papers)</th>
</tr>
</thead>
<tbody>
<tr>
<td>NGC 6543</td>
<td>0.95</td>
<td>----</td>
<td>1.00f</td>
<td>0.24</td>
<td>1.5h</td>
</tr>
<tr>
<td>NGC 6572</td>
<td>1.13</td>
<td>2.0a</td>
<td>0.67a</td>
<td>0.97</td>
<td>1.0h</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>0.75f</td>
<td></td>
<td></td>
</tr>
<tr>
<td>NGC 7009</td>
<td>1.13</td>
<td>----</td>
<td>0.67a</td>
<td>0.97</td>
<td>0.6h</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>0.64i</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>1.0j</td>
</tr>
<tr>
<td>NGC 7027</td>
<td>1.55</td>
<td>2.22b</td>
<td>0.72b</td>
<td>0.77</td>
<td>0.5i</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>0.8j</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>2.0j</td>
</tr>
<tr>
<td>NGC 7662</td>
<td>1.3</td>
<td>2.86c</td>
<td>0.74g</td>
<td>0.70</td>
<td>0.6j</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>0.63c</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>0.9h</td>
</tr>
<tr>
<td>IC 418</td>
<td>1.83</td>
<td>2.50d</td>
<td>0.83a</td>
<td>0.56</td>
<td>2.0j</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>1.6h</td>
</tr>
<tr>
<td>Orion (NGC 1976)</td>
<td>0.90</td>
<td>2.16e</td>
<td>0.75a</td>
<td>0.70</td>
<td>1.2i</td>
</tr>
</tbody>
</table>
C. Discussion

The general approach of solving atomic rate equations to determine various parameters is not new. In fact, considerable work has been done along this line for hydrogen, helium and oxygen. A detailed study of abundance equilibrium for sulphur, as given in this thesis, hopefully affords yet another means of analyzing the spectra of astrophysical objects, and aids in a more complete understanding of them. The extent to which the SII data can be used to study objects such as novae remnants, T-Tauri stars, HII regions and perhaps even quasars has not been pursued by the author although these research directions show promise.
VI. ACKNOWLEDGEMENTS

I am pleased to acknowledge the stimulating discussions that I have had with my advisor, Dr. Donald D. Clayton. His advice and encouragement have been most helpful in the conduct of my research.

The origins of this thesis developed during numerous conversations which the author had with Dr. H.C. Goldwire in the summer of 1967. Subsequent talks with Drs. Clayton, N. Lane, and R.A. Wolf have aided in bringing the solution of the problem to its present status.

For the past two years the author has been the recipient of a National Defense Education Act Fellowship. Additional research funds were obtained from the National Science Foundation under GP-8174.

Finally, I wish to express appreciation to my wife, Janet, who typed both the rough and final drafts of this thesis. Without her assistance and understanding this work would not have evolved.
VII. REFERENCES


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_______, 1962, private communication with C.W. Allen;
results published in Astrophysical Quantities.


APPENDIX A: INELASTIC ELECTRON-ATOM CROSS SECTIONS

As noted in Section II, the cross section $Q(i,j)$ for an inelastic electron-atom collision can be written as

$$Q(i,j) = \frac{\pi}{k^2} \frac{\Omega(i,j)}{\omega_i} .$$  \hspace{1cm} (A.1)

$k$ is the incident electron's wave number, and $\omega_i$ is the degeneracy of the initial atomic state. The concept of a collision strength, $\Omega(i,j)$, obtains from the following argument. Classically, the colliding electron's path is characterized by an impact parameter $s$, which is the distance of closest approach for an undeflected trajectory. If the probability of the transitions $(i)\rightarrow(j)$ occurring for a given impact parameter is $P(i,j;s)$, it is possible to express the cross section

$$Q(i,j) = \int_0^\infty P(i,j;s)2\pi s ds .$$  \hspace{1cm} (A.2)

Now $s$ is related to the angular momentum of the electron, $L$, by

$$L = mvs .$$  \hspace{1cm} (A.3)

If the angular momentum is quantized,

$$s_L = \frac{1}{mv}[\ell(\ell + 1)\pi^2]^{1/2}$$  \hspace{1cm} (A.4)

and, as a result, the integral (A.2) becomes a summation over all possible $\ell$ values:
2sds → (2l + 1)h^2 / (mv)^2 = (2l + 1)/k^2 \quad (A.5)

and then

Q(i,j) = \sum_{l=0}^{\infty} \frac{\pi}{k^2} (2l + 1)P(i,j; s) \quad (A.6)

For degenerate states, the cross section is weighted by the statistical weight of initial term. It follows then that the collision strength

Ω(i,j) = \sum_{l=0}^{\infty} (2l + 1)P(i,j; s) \quad (A.7)

Seaton (1958) has shown that if one assumes L-S coupling in both initial and final states, collision strengths for transitions between spectral terms

\[ \Omega(\alpha L S, \alpha'L'S') = \frac{1}{2} \sum_{\ell} \frac{T^T_{ST}}{S_L^T} (2S^T + 1)(2L^T + 1) \times \]

\[ |S(\alpha, S_L S^T_{L}; \alpha' S'L' S^T_{L'})|^2. \quad (A.8) \]

The notation is:

- \( S^T, L^T \) - total spin and total orbital angular momenta;
- \( \ell', \ell \) - incident and outgoing electron orbital angular momenta;
- \( S(\quad) \) - scattering matrix element.

To obtain \( \Omega(\alpha S L J, \alpha'S'L'J') \), a transformation of the matrix representation to one involving \( J^T \) must be effected. This is possible through the use of vector coupling coefficients.
(9-j symbols).

\[ S(\alpha, SLJ; \ell, S'L'J'; \alpha', S'L'J') = \]

\[ \sum_{S_{LT}T} \left[ \begin{array}{ccc} L & S & J \\ \ell & 1/2 & j \\ S_{LT} & T & S_T & J_T \end{array} \right] S(\alpha, SLJ; \ell, S'L'J'; \alpha', S'L'J') x \]

\[ A \left[ \begin{array}{ccc} L' & S' & J' \\ \ell' & 1/2 & j' \\ L_T & S_T & J_T \end{array} \right] \]

(A.9)

Equation (A.9) can be used to obtain (Seaton, 1958)

\[ \Omega(\alpha, SLJ; \alpha', S'L'J') = \]

\[ \frac{1}{2} \times \sum_{\ell\ell'} \left| S(\alpha, SLJ; \ell, S'L'J'; \alpha', S'L'J') \right|^2 \quad (A.10) \]

The S-matrix elements for the transitions to be considered here can be calculated more easily if the following approximations are employed:

1) Because all terms involved arise from the same configuration, strong coupling should exist only for certain values of \( \ell \) and \( \ell' \). In fact, Seaton (1958) has shown that for the \( 3p^3 \) configuration \( \ell = \ell' = 1 \) is the only partial wave that contributes significantly to the cross section.

2) If an exact resonance approximation is used for the \( \ell = \ell' = 1 \) close coupling case, and a distorted wave approximation is used for \( \ell = \ell' \neq 1 \) (weak...
coupling), the S-matrix elements may be computed with some accuracy by treating all other interactions as perturbations.

Further discussion of these topics may be found in Mott and Massey (1965) and Moiseiwitsch and Smith (1968).
APPENDIX B: GENERAL THEORY OF ATOMIC PHOTOIONIZATION

The ionization of an atom may be viewed in part as a transition from a system containing \( n \) photons to one containing \( n-1 \) photons. To be treated by ordinary quantum mechanical perturbation theory, the perturbation causing the transition - the interaction of an electron with an electromagnetic field - must be small. The Hamiltonian for a system consisting of an electron plus an electromagnetic field may be written

\[
H = H_e + H_f = \frac{1}{2m} \left[ -i\hbar \vec{\nabla} - e\vec{A} \right]^2 + e\phi + \sum_\omega (n_\omega + 1/2)\hbar \omega \quad (B.1)
\]

\( \vec{A} \) and \( \phi \) are vector and scalar potentials specifying the field, and the third term is the sum of the energies of photons with angular frequency \( \omega \). This term obtains from a Fourier expansion of the vector potential

\[
\vec{A} = \sum_\omega \left[ q_\omega(t)\vec{A}_\omega(\vec{x}) + q^*_\omega(t)\vec{A}^*_\omega(\vec{x}) \right] \quad (B.2)
\]

and subsequent recognition of the Hamiltonian of a field component as that of a simple harmonic oscillator. By substituting Equation (B.2) into Equation (B.1), that part of the Hamiltonian representing the interaction of the particle and the field is found to be:

\[
H_{\text{int}} = \frac{ie\hbar}{m} \vec{\nabla} \cdot \sum_\omega \left[ q_\omega \vec{A}_\omega + q^*_\omega \vec{A}^*_\omega \right]
\]

\[+ \frac{e^2}{2m} \sum_{\omega, \omega'} \left[ q_\omega q^*_\omega \vec{A}_\omega \cdot \vec{A}^*_\omega, + q_\omega q^{*^2} \vec{A}_\omega \cdot \vec{A}^*_\omega, \right.
\]

\[+ q^*_\omega q_\omega \vec{A}^*_\omega \cdot \vec{A}_\omega, + q^*_\omega q^{*^2} \vec{A}^*_\omega \cdot \vec{A}^*_\omega, \] \quad (B.3)

-60-
The usual techniques of perturbation theory may be applied to solve Schrödinger's equation involving the Hamiltonian in Equation (B.1). Expanding the solutions $|\psi_f\rangle$ in terms of a complete set of "unperturbed" solutions, {$|\psi_i\rangle$},

$$|\psi_f\rangle = \sum_i a_{fi}(t)|\psi_i(t)\rangle$$

$$= \sum_i a_{fi}(t) \exp\left[-\frac{iE_i t}{\hbar}\right]u_i(x)$$

one calculates that

$$|a_{fi}(t)|^2 = 2 \frac{|\langle\psi_f|H_{\text{int}}|U_i\rangle|^2}{(E_f-E_i)^2} \left[1-\cos\left(\frac{E_f-E_i}{\hbar} t\right)\right]$$

is the probability of finding the system, initially in state $|\psi_i\rangle$, in state $|\psi_f\rangle$ at a later time $t$. If the transitions of interest can leave the system in any one of several, almost identical, final states, the total transition probability $P_{fi}$ is

$$P_{fi} = \sum_{f'} |a_{f'i}(t)|^2 = \int |a_{f'i}(t)|^2 \rho(E_{f'}) dE_{f'},$$

where $\rho(E_{f'})$ is the density of final states in the interval $E_{f'}$, $E_{f'}+dE_{f'}$. The integral (B.6) has a sharp maximum at $E_{f'} = E_i$, so if the matrix element between initial and final states, and the density of states do not vary too rapidly, one can set

$$P_{fi} \approx \frac{2\pi}{\hbar} |\langle\psi_f|H_{\text{int}}|U_i\rangle|^2 \rho(E_f)$$

Equation (B.7) is valid so long as the time involved is short
enough to justify the use of perturbation techniques. For the problem considered here, photoionization, all quantum numbers of the initial and final states are specified. The density of states is just a delta function involving the electron's and photon's energies,

$$\rho(E_f) = \delta(n\omega - \chi - Z^2\varepsilon) \quad (B.8)$$

which insures energy conservation.

When photoionization occurs, the initial state and final state are characterized by the number of photons, $|n\rangle$ and $|n-1\rangle$. The properties of $q^w$ and $q^w^*$ are such that they have non-zero matrix elements (in this $|n\rangle$ representation) only when photons are "created" or "annihilated", respectively. These properties are demonstrated explicitly by the relations (Griem, 1964):

$$\langle n_w | q_w | n_{w'} + 1 \rangle = \delta_{w,w'} \delta_{w,w''} \left[ \frac{n_w}{2\omega} (n_w + 1) \right]^{1/2} e^{-i\omega t} \quad (B.9a)$$

$$\langle n_w + 1 | q_w^* | n_w^{''*} \rangle = \langle n_w + 1 | q_w^* | n_w^{''} \rangle = \delta_{w,w'} \delta_{w,w''} \left[ \frac{n_w}{2\omega} (n_w + 1) \right]^{1/2} e^{i\omega t} \quad (B.9b)$$

$$\langle n_w + 1 | q_{w}^* | n_w^{''} + 1 \rangle = \langle n_w | q_w^* | n_w^{''} + 1 \rangle = 0 \quad (B.9c)$$

The vector potential satisfies the homogeneous wave equation and the Lorentz condition; it follows then, that the individual Fourier components can be expressed

$$\vec{A}_\omega = \vec{A}_\omega^0 e^{i\vec{k} \cdot \vec{r}} \quad (B.10)$$
\[ \tilde{A}_\omega^0 \text{is the amplitude of } \tilde{A}_\omega \text{ associated with a photon of frequency } \omega, \text{ and satisfies } \tilde{A}_\omega^0 \cdot \vec{k} = 0. \vec{k} \text{ is the propagation vector for the photon.} \]

The energy in the field due to an oscillation frequency \( \omega \) is

\[
(n_\omega + 1/2)\hbar \omega = \frac{1}{2} \int (\vec{E}_\omega \cdot \vec{D}_\omega + \vec{B}_\omega \cdot \vec{H}_\omega) \, d\tau \tag{B.11}
\]

\[
= (n_\omega + 1/2)\hbar \omega \varepsilon_0 \tilde{A}_\omega^0 \cdot \tilde{A}_\omega^0 L^3
\]

if the integration is over a volume \( L^3 \). Then

\[
\tilde{A}_\omega^0 = \varepsilon_0^{-1/2} \frac{1}{A} \frac{\hbar}{\alpha}
\tag{B.12}
\]

where \( \vec{a} \cdot \vec{a} = 1, \vec{a} \cdot \vec{k} = 0. \)

Employing the above relations the matrix element

\[
\langle \psi_f | H_{\text{int}}| \psi_i \rangle
\]

can be calculated. For simplicity let \( |\psi_f\rangle \rightarrow |f\rangle \) and \( |\psi_i\rangle \rightarrow |i\rangle \). Then since \( |i\rangle \) represents a system with one more photon than \( |f\rangle \), only the terms

\[
\varepsilon_0^{-1/2} \frac{1}{A} \frac{\hbar}{\alpha} \sum_\omega \langle f | \frac{ie\hbar}{m} \vec{v} \cdot \vec{a} e^{-i\vec{k} \cdot \vec{r}} q_\omega | i \rangle
\tag{B.13}
\]

do not vanish. The photoelectric cross section, denoted \( \alpha_{fi} \), is the probability for the transition divided by the flux of incident photons. If there is 1 photon in the volume \( L^3 \), with an angular frequency \( \omega = (Z^2 e^+ \chi) / \hbar \),

\[
\alpha_{fi} = \frac{L^3}{c} \frac{2\pi}{\hbar} \frac{1}{\varepsilon_0 A L^3} \left| \langle f | \frac{ie\hbar}{m} \vec{v} \cdot \vec{a} e^{-i\vec{k} \cdot \vec{r}} q \rangle | i \rangle \right|^2
\]

\[
= \left( \frac{2\pi \varepsilon_0^2 A L^3}{e_0 cm^2} \right) \left| \langle f | \vec{v} \cdot \vec{a} e^{-i\vec{k} \cdot \vec{r}} q \rangle | i \rangle \right|^2
\tag{B.14}
\]
If \( \exp(-ik \cdot r) \) is expanded keeping only the first term - the dipole approximation - and the Equations (B.9) employed \( (n_i = 1) \), Equation (B.14) reduces to

\[
\alpha_{fi} = \left( \frac{2\pi e^2 \hbar}{\epsilon_0 c m^2} \right) \left( \frac{\hbar}{2\omega} \right) |\langle f \mid \vec{V} \cdot \vec{a} \mid i \rangle|^2 . \tag{B.15}
\]

The matrix element now involves only the particle's coordinates.

The gradient operator \( \vec{V} \cdot \frac{i}{\hbar} \vec{P} = i \frac{\hbar}{m} \vec{r} = i \frac{\hbar}{m} \vec{r} \omega \), thereby allowing the cross section to be written

\[
\alpha_{fi} = \frac{\pi e^2 \omega}{\epsilon_0 c} |\langle f \mid \vec{r} \cdot \vec{a} \mid i \rangle|^2 . \tag{B.16}
\]

Averaging over all possible orientations of the absorbing system the cross section can finally be expressed as

\[
\alpha_{fi} = \frac{\pi e^2 \omega}{3\epsilon_0 c} \sum_j |\langle f \mid x_j \mid i \rangle|^2 . \tag{B.17}
\]

If there is more than one initial state and/or final state of fixed energy, \( \omega_i \) being the degeneracy of the initial state,

\[
\alpha_{fi} = \frac{\pi e^2 (2\pi \nu)}{3\epsilon_0 c \omega_i} \sum_j' |\langle f \mid x_j \mid i \rangle|^2 , \tag{B.18}
\]

where \( \sum' \) indicates a summation over all of these state, initial and final. A quantity \( S \) may be introduced so that

\[
\alpha_{fi} = \frac{4\pi a_0^2}{3} (\chi + Z^2 \epsilon) \frac{S}{\omega_i} . \tag{B.19}
\]

\( \alpha \) and \( a_0 \) are the fine structure constant and Bohr radius, respectively, and
Assuming L-S coupling, the initial and final states can be specified by appropriate quantum numbers

\[ |i\rangle = |\xi;L,S,M\rangle; \quad (B.21a) \]

\[ |f\rangle = |\xi'';L''S''M''S',L'S'M'M',k\ell'\rangle. \quad (B.21b) \]

The double prime refers to the ion and the single prime refers to the system of ion plus ejected electron of orbital angular momentum \( \ell' \).

If the ejected electron's state function is taken orthogonal to all bound state functions, and each of the other electrons is assumed to have a state function unchanged by the ionization, then

\[
\frac{S}{\omega_i} = \sum_{\ell' = \pm 1} \sum_{L' = L, L' \pm 1} C_{\ell'L'} \int_0^\infty \left| P_n, l'(r) G_{k\ell'}(r) \right|^2 dr \quad (B.22)
\]

\( \frac{1}{r} G_{k\ell'}(r) \) and \( P_{n\ell}(r) \) are radial portions of the ejected \((k\ell')\) electron's and bound \((n\ell)\) electron's state functions. The \( C_{\ell'L'} \) 's are algebraic factors arising from integrations over spin and angular coordinates. The ranges of the two summations are due to the usual dipole selection rules:

\[ S = S'; \quad S = S'; \quad L = L', L' \pm 1; \quad M_L = M_L', M_L' \pm 1. \]

For the photoionizations of interest here, one of three (SII) or four (SI) equivalent 3p electrons is ejected. As a
consequence, the $C_{q'L'}$'s have the form ($q = 3$ or $4$):

$$C(q^SL \rightarrow q^{q-1}S'L'' ; S'L' l') = (2l+1)(2l'+1)W^2(l l' LL'' ; LL'') C(q^SL \rightarrow q^{q-1}S'L'' ; l')$$

The $C(q^SL \rightarrow q^{q-1}S'L'' l')$ coefficients have been tabulated in Burgess and Seaton (1960) and Griem (1964); the $W$'s are Racah coupling coefficients. The $C_{q'L'}$'s used are tabulated in TABLE II.4. Note that the following relations hold:

$$C(q^SL \rightarrow q^{q-1}S'L'' ; l') = \sum_{L'} C(q^SL \rightarrow q^{q-1}S'L'' ; S'L' l')$$

and

$$C(p^SL \rightarrow p^{p-1}S'L'' ; l') = 2C(p^SL \rightarrow p^{p-1}S'L'' ; l')$$