ANALYSIS OF THE Si II AND Si III DR PROCESSES APPLIED TO STELLAR ENVELOPES

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ABSTRACT

In an earlier attempt to explain the observed excess in the IR flux of Be stars, we have analyzed the dielectronic recombination (DR) of Mg II in stellar envelopes and the influence of this atomic process on the stellar flux. In the present paper, we study the DR of other ions with astrophysical significance, namely, Si II and Si III, and reach the conclusion that Si II may also contribute to the IR excess in Be stars.

Subject headings: atomic processes — infrared: stars

1. INTRODUCTION

In earlier papers (Cruzado, Di Rocco, & Ringuelet 1998, hereafter PI; Cruzado & Ringuelet 2000, hereafter PII), we have discussed the significance of the dielectronic recombination (DR) of Mg II, which takes place in the cool stellar envelope of early-type stars, to the emitted IR excess. Following an electron capture by Mg II atoms in the ground state, Mg I atoms form in *autoionizing levels* above the first ionization limit, and a cascade process to lower bound levels does give rise to emission lines, the energy emitted in those lines contributing to the observed IR excess.

We have considered three rather well-defined regions in the atmospheres of Be stars (see §§ 2, 3, and 6 of PI): a photosphere in radiative and hydrostatic equilibrium, a chromosphere, thin in size, where the temperature of the expanding material increases, and an expanded cool envelope where the temperature has a constant low value and the electron density decreases smoothly. *T*-values (temperature) usually adopted for this outer layer are in the range 5×10^3 to 10^4 K, and $10^7 \le N_e \le 10^{11}$ is consistent with our atmospheric model. These physical conditions in cool stellar envelopes are favorable to the DR process.

The significance of the DR in low-density media, at high and low temperatures, has been already emphasized by several authors (Burgess & Seaton 1964; Nussbaumer & Storey 1983, 1984, 1986). Atoms of any element, except H II, being ionized at least once, could undergo DR. The emissivity in a line whose upper level is populated by DR is proportional to the number of atoms being recombined, and the energy emitted in this line will be significant only if the number of ions undergoing recombination is large enough. In addition, that number will depend on (1) the cosmic abundance of the element and (2) the ionization balance, which in turn depends on the ionization potential of the ionic species and on the physical conditions in the medium. It is clear that, for the values of electron density and temperature generally adopted for the outer layers of the cool stellar envelopes in Be stars (see §§ 2–3 of PI), Mg II, Si II, and Fe II are the elements to be considered. We first took up the DR of Mg II (PI) because of the simple atomic structure of the Mg I atom resulting from the recombination process. In the present work, we will attempt to analyze the DR of Si II.

In addition, we will try to determine the importance of the contribution to the IR stellar flux of the DR of Si III. In the case of Si III, we have to consider that this process may occur in deeper layers of the stellar envelope, i.e., in regions closer to the central star, where we will have to take into account other physical processes competing with DR.

2. DR OF Si п

2.1. About the Si I Atomic Structure

The electron configuration of a Si I atom in the ground state is $1s^22s^22p^63s^23p^2$. The fact that in such a case we have four electrons outside a closed shell readily indicates that the study of the DR of Si II will be more complicated than that of Mg II. In fact, a very large number of transitions occurs among the many energy levels that originate in excited configurations. Moreover, the excitation of an outer electron gives rise to series of energy levels converging on two different limits: Si II $3s^23p^2P_{1/2}^0$ (hereafter ${}^2P_{1/2}^0$), at 65,747.76 cm⁻¹ from the ground state, and Si II $3s^23p^2P_{3/2}^0$ (hereafter ${}^2P_{3/2}^0$), at 66,035.00 cm⁻¹ from the ground state. This occurs because of the doublet structure of the first ionization limit of the Si I atom (see Fig. 1). In addition, there are levels resulting from the excitation of one outer electron that lie above the lower of the two components of the doublet and could also be autoionizing levels.

In order to decide if these levels could undergo autoionization, we have to consider the coupling schemes of the terms and also the selection rules for the process. From this analysis, we conclude that all states between the components of the doublet are able to autoionize in LS coupling, except those originating in the terms ${}^{1}S^{0}$ and ${}^{3}S^{0}$ belonging to the $3s^{2}3pnp$ configurations. However, because of departures from LS coupling by these high series members, these levels are strongly coupled to

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FIG. 1.—Grotrian diagram showing the energy level structure of the Si I atom. The levels in the boxes are the ones we selected to perform the calculations.

states able to autoionize, and consequently we can also consider them to be autoionizing levels, with $P^A > P^R$, P^A being the autoionization probability and P^R the radiative probability.

With regard to the configurations with two excited electrons that generate levels above ${}^{2}P_{3/2}^{0}$, only the $3s3p^{3}$ configuration gives rise to states lying energetically close to ${}^{2}P_{3/2}^{0}$ (in order to be reached by the free electron at the low temperature considered here). Among theses states there are some that are able to autoionize in LS coupling: precisely those closest to ${}^{2}P_{3/2}^{0}$. The $3s3p^{3}$ configuration also gives rise to bound states below ${}^{2}P_{1/2}^{0}$.

2.2. Methodology

In the present study, the methodology that we have followed is, in general, the same as that used for Mg, as described in PI; however, in the case of Si, the software and the computer limitations introduce larger constraints on the calculation. Cowan's code was used to calculate atomic parameters; this code is a set of FORTRAN 77 programs for the calculation of radial wave functions of a spherically symmetrized atom and several radial integrals involved in the calculation of atomic energy levels and spectra. A brief description of the programs is given by Cowan (1981). Only a limited number of configurations may be handled with Cowan's code; therefore, we must perform a suitable selection of these configurations, in order to obtain representative results. To do so we have to take into account the level structure of the Si I atom and the physical conditions in the region where the DR takes place.

In an atom having a simple ionization limit, such as Mg I, there are configurations that generate bound levels and those that generate autoionizing levels, with a few exceptions, such as $3p^2$ in Mg I, that generate both kinds of levels. In the case of Si I, in order to select the atomic configurations to work with, we also have to consider (1) bound levels with principal quantum number smaller than a critical value, n_0 , which will be set by taking into account the electron density in the medium, and (2) bound levels with $n > n_0$ that will be depopulated by collisional transitions before a radiative transition takes place (see § 6 of PI). Moreover, radiative transitions between levels with large n lying very close to each other give rise to emitted energy at wavelengths much larger than the IR wavelength we are interested in. In addition, because the level density increases as n increases, if the levels involved in the transition are not very close to each other, the resulting Δn may be large enough to imply a small amount of emitted energy. In the case of the autoionizing levels, a value of n'_0 will be imposed by the local temperature in relation to each particular atom, the temperature will determine the value of ΔE (energy above the ionization limit) reached by the free electrons, and the corresponding principal quantum number will depend on the autoionizing level density in the atom.

The Si I atom, however, requires a more exhaustive analysis. In this atom, each atomic configuration with one outer excited electron gives rise to levels that belong to a series with the ${}^{2}P_{1/2}^{0}$ limit and to levels that belong to a second series with the ${}^{2}P_{3/2}^{0}$ limit. Thus, for a large enough value of *n*, both bound and autoionizing levels will be generated by the same configuration.

As a consequence, we have proceeded as follows. In a first step, we considered configurations $3s^23pns$, $3s^23pnp$, $3s^23pnd$, and $3s^23pnf$, which originate with the excitation of one outer electron and have $n \le 22$, and the configuration $3s^3p^3$. With a table of experimental energy levels at hand, we verified that the autoionizing levels lying between ${}^2P_{1/2}^0$ and ${}^2P_{3/2}^0$ have $n \ge 20$ (see Fig. 1).

Because of the high level density between the doublet components, levels with n = 22 are at no more than 100 cm⁻¹ above the ionization limit $({}^{2}P_{1/2}^{0})$, a quantity surpassed by free electrons at the temperature considered; as a consequence, it seems that n = 22 is insufficient. On the other hand, we have verified that bound levels with $n \ge 10$ have no influence on the final results; consequently, we can ignore the configurations with $10 \le n \le 20$ and introduce other configurations with $n \ge 22$.

In a second step, we used configurations $3s^23pns$, $3s^23pnp$, $3s^23pnd$, and $3s^23pnf$, both with $n \le 10$ and with $20 \le n \le 27$, as well as configuration $3s^2p^3$ (see Fig. 1). With this group of configurations many calculations were carried out, in order to



FIG. 2.—Flux distribution vs. wavelength for three different values of the electron temperature, 3000, 5000, and 7000 K. For all curves the electron density has the same value, 10^8 particles cm⁻³. The value adopted for the emitting volume was $98V^*$ (V^* = stellar volume). BB represents the photospheric flux and DR is the flux due to DR of Si II.

determine the contribution of each one to the flux and to analyze the behavior the flux as a function of electron density N_e , electron temperature T_e , and emitting volume V.

2.3. Results

In Figure 2 we show some of our results, plotting the flux distribution against wavelength for sets of values of N_e and V; different curves correspond to different values of T_e .

As the temperature increases, more and more autoionizing levels are reached by the free electrons, and the DR becomes more and more effective. But when the number of recombining ions starts to decrease, the process is weakened. We determined that the contribution to the flux of the autoionizing levels with $n \ge 25$, as well as that of the autoionizing levels originating in the $3s3p^3$ configuration, can be neglected for the temperatures considered here. We must point out that electron capture by Si II atoms may occur at very low temperatures because of the location of the first autoionizing level, which is actually very close to the first ionization limit (see the Appendix for further comments).

For the values of electron density considered here, the bound levels that depopulate by radiative decay before a collisionally induced process occurs are the ones with n < 30. Nevertheless, as we have said in § 2.2, bound levels with n > 10 have no influence in the emergent flux for the electron density considered in this work. Thus, the resultant flux is practically proportional to the value of N_e , provided that this value is lower than 10^{12} particles cm⁻³.

3. DR OF Si III

To analyze the DR of Si II, we have adopted an atmospheric model proposed by Ringuelet, Fontenla, & Rovira (1981) and developed by Thomas (1983) (see § 2 of PI). DR of Si II would take place in the outer region of this atmosphere, where the temperature has a constant low value and the electron density decreases smoothly; thus, the geometric thickness of the region where the process occurs may be rather large. In an inner region, where the temperature is higher, DR of other elements or ions could occur. The process will be effective if the number of recombining atoms is large enough and if the electron density is not very high. However, in a region closer to the star, we must consider that the induced radiative transitions, as well as the opacity of the media, could influence the results. On the other hand, the geometric thickness of this region cannot be very large because of its large temperature and density gradient.

3.1. Transparent Medium and Diluted Radiation Field

We considered the configurations $3s^2ns$, $3s^2np$, $3s^2nd$, and $3s^2nf$ with $n \le 10$ that give rise to bound levels, the configurations 3s3p4s, 3s3p4p, 3s3p4d, and 3s3p4f that give rise to bound and autoionizing levels, and the configuration $3p^3$ that generates autoionizing levels. In addition, because of the strong mixing of configurations, we had to take into account configurations $3p^2ns$, $3p^2np$, $3p^2nd$, and $3p^2nf$ with $n \le 10$. When we compared the energy levels obtained via Cowan's code with those obtained experimentally, we noted a strong interaction between the $3s^2ns$ series and the $3p^2ns$ series, as well as between the $3s^2np$ series and the $3p^2np$ series, and so on.

Working with this group of configurations and assuming a transparent region and a very diluted field, we obtain the curve shown in Figure 3.



FIG. 3.—Flux distribution vs. wavelength for $T_e = 10,000$ K, $N_e = 10^9$ particles cm⁻³, and two different values of the emitting material volume, $V = 6V^*$ and $V = 98V^*$. BB represents the photospheric flux and DR is the flux due to DR of Si III.

We may predict that the configurations giving rise to bound levels with $n \ge 10$ (not considered at present) will produce, in addition, a flux excess that will be noticeable for $\lambda \ge 10 \mu$.

3.2. Adding Induced Radiative Transitions

3.2.1. Autoionizing Levels

In order to obtain the recombination coefficient for Si II (which is formed in the same region as Mg II), we solved the statistical equilibrium equations by assuming that an autoionizing level could be populated only by electron capture and depopulated by autoionization or by downward radiative transitions. In the case of Si III, we have taken into account induced radiative transitions as processes populating or depopulating an autoionizing level.

In order to evaluate the influence of the new terms in the statistical equilibrium equations, we took into account that, for light atoms, the autoionization processes occur much more frequently than the radiative ones, because the autoionization probability is nearly independent of the atomic number, whereas the radiative transition probability increases as the fourth power of the atomic number (Condon & Shortley 1953; Nussbaumer & Storey 1986). If we estimate the relative significance of the different terms, we conclude that induced radiative transitions affect to a very small extent the population of the autoionizing levels.

3.2.2. Bound Levels

By assuming that a bound level can be populated or depopulated only by spontaneous radiative transitions, we obtain for a line with the wavelength λ_{lh} an emissivity value of

$$f(\lambda_{lh}) = \frac{N_e N^{\rm S} \sum_{j} \left[(g_j/2g_m) (h^2/2\pi m KT)^{3/2} e^{-E_j/KT} P_{jh}^{\rm R} \right]}{\sum_{k < l} P_{lk}^{\rm R}} P_{lh}^{\rm R} h v_{lh} , \qquad (1)$$

where *j* represents autoionizing states of the Si II atom, *l*, *h*, and *k* are bound states of the Si II atom, E_j is the energy of the *j* state above the first ionizing limit, P_{jh}^R , P_{lh}^R , and P_{lk}^R represent the probabilities for the $j \rightarrow h$, $l \rightarrow h$ and $l \rightarrow k$ radiative transitions (s⁻¹), N_e is the number of electrons per unit volume, and N^S is the number of Si III atoms given by the Saha equation. The rest of the symbols have their usual meaning.

If the bound level is populated or depopulated by induced radiative transitions—in addition to the spontaneous radiative ones—the emissivity in the line may be modified. The emissivity in the line must then be expressed as

$$\epsilon(\lambda_{lh}) = \frac{N_e N^{\rm s} \sum_{j} \left[(g_j/2g_m) (h^2/2\pi m KT)^{3/2} e^{-E_j/KT} P_{jh}^{\rm R} \right] + \sum_{k \neq l} P_{kl}^{\rm Ri} J N_k}{\sum_{k < l} P_{lk}^{\rm R} + \sum_{k \neq l} P_{lk}^{\rm Ri} J} P_{lk}^{\rm Ri} J \qquad (2)$$

Here, the additional term in the numerator represents all induced radiative transitions populating the upper level, and the additional term in the denominator takes into account the induced radiative transitions depopulating this level. P_{kl}^{Ri} and P_{lk}^{Ri} represent the probabilities for the $k \rightarrow l$ and the $l \rightarrow k$ induced radiative transitions, J represents the radiation field at the distance D from the star, and N_k is the number of Si II atoms in the k state.





FIG. 4.—Flux distribution vs. wavelength for $T_e = 10,000$ K, $N_e = 10^9$ particles cm⁻³, and $V = 98V^*$. In one of these curves the radiative induced transitions depopulating the upper line levels were considered. Although $V = 6V^*$ would be a more suitable value, we have adopted $V = 98V^*$ in order to make more evident the discrepancy between the curves.

In order to calculate this expression we need the population levels (N_k) , which are not immediately available. Nevertheless we may estimate the influence of the induced radiative transitions on the emitted flux in the following ways.

First, we assume that the contribution of the induced transitions populating the upper level is negligible, which is equivalent to setting $\sum_{k \neq l} P_{kl}^{Ri} JN_k$ to 0; then, equation (2) becomes

$$\epsilon(\lambda_{lh}) = \frac{N_e N_s \sum_j \left[(g_j/2g_m) (h^2/2\pi m KT)^{3/2} e^{-E_j/KT} P_{jh}^R \right]}{\sum_{k \le l} P_{lk}^R + \sum_{k \ne l} P_{lk}^{Ri} J} P_{lh}^R h v_{lh} .$$
(3)

The resultant flux would be the one displayed in Figure 4, where two curves are drawn by using equations (1) and (3), respectively. As expected, the effect of the induced radiative transitions depopulating the bound levels is to reduce the resultant flux, and this effect is very small for a temperature of 10,000 K at $5R_{\star}$ from the star.



FIG. 5.—Flux distribution with wavelength for $T_e = 10,000$ K, $N_e = 10^9$ particles cm⁻³, and $V = 98V^*$. In one of these curves all the radiative induced transitions populating and depopulating the upper line levels were considered.



FIG. 6.—On a temperature-density diagram, $\tau = 1$ curves for four different wavelengths. L is the geometrical depth and e-column is the column of the electrons.

Second, we solved equation (2) by assuming a Boltzmann distribution for the level populations. In Figure 5 we can see that the modification of the resultant flux is due almost entirely to the induced radiative transitions that populate the bound levels: the effect could be considerable. If the level population numbers are obtained by assuming distributions other than the Boltzmann distribution, the effect would always be to increase the emergent flux.

3.3. Nontransparent Medium

Concerning the possible influence of the opacity of the medium on the emitted flux, we recall the discussion in PII, where, in considering the continuum opacity of the envelope, we had taken into account the bound-free and the free-free transitions in hydrogen atoms and negative ions of hydrogen, together with Rayleigh-Thomson scattering. In PII the behavior of the opacity with respect to electron density, temperature, and wavelength is shown.

We summarize and illustrate the conclusions obtained in that study in Figure 6, where we have drawn $\tau = 1$ curves on a temperature-density diagram to estimate how appropriate it is to adopt a transparent medium. We have evaluated $\tau = 1$ for two different values of L, the geometric thickness of the region whose opacity is calculated. Each curve, for different wavelengths, separates two regions: a transparent region below and an opaque region above. It can be seen that, when the temperature is below 6000 K, the medium becomes opaque for density values lower than 10^{12} , and the opacity increases at very short and very long wavelengths, as discussed in PII. On the other hand, when the temperature is higher than 6000 K, the larger the opacity value.

Unlike the DR of Mg II and Si II, the DR of Si III takes place in a region located close to the star. The energy originated in the DR of Si III has to pass through many layers with different temperatures and densities, where the opacity may be important. Although we have not adopted a specific model to treat the radiative transfer problem strictly, we suggest that the opacity effect will be important at very short and very long wavelengths.

4. CONCLUSIONS

The contribution of the DR of Si II to the emitted flux at IR wavelengths is very important. No excess is obtained in the UV region.

We should emphasize the large increase in the flux caused by this process at $\lambda = 5 \mu$, which corresponds to the *M* band: by adopting for *T* a value of 5000 K, for N_e a value of 10⁸, and for *V* a value of 98*V**, an excess flux of 6 mag was obtained at $\lambda = 5 \mu$ (Fig. 2). In this regard, an anomalous 5μ point observed in some Be stars is discussed by Woolf, Stein, & Strittmatter (1970). In spite of the approximations made in the calculations, we think that a large excess flux at this wavelength will be observed even if a more specific model is adopted.

We think that the whole excess flux of every Be star cannot be explained by taking into account only one atomic process. One should include free-free and free-bound processes and the DR of several atomic species, each process contributing separately. For example, regarding the anomalous flux at 11.5 μ also discussed by Woolf et al., we find that an important flux excess appears to result at this wavelength from the DR of Mg II (see PI).

On the other hand, the DR of Si III has little influence on the flux; because of the large gradient in temperature and density where it occurs, the region with suitable physical conditions to make the process effective will be small. In Figure 3, we can see that if a value of $6V^*$ is adopted for that region the resulting contribution is a very poor one. In addition, the opacity plasma may be important. Perhaps some excess may remain at the wavelength interval of the *R* band, where the energy emitted as a

result of the DR of Si III has an important value. We believe that the contribution to the flux will come, mainly, from the ions that are abundant enough in the outer layers of the stellar atmosphere, and to ascertain this possibility an analysis of the possible influence of the DR of Fe II is in progress.

APPENDIX

We add a comment in regard to a suggestion made earlier by Underhill (1981). She attributes to the DR process the broadening of the Si II $\lambda\lambda 1305.6$ and 1309.6 lines that are observed on IUE spectra of Be stars and correspond to the transitions $3s_3p^2 {}^2D_{5/2} \rightarrow 3s_3p_3d {}^2F_{7/2}^0$, $3s_3p^2 {}^2D_{5/2} \rightarrow 3s_3p_3d {}^2F_{5/2}^0$, and $3s_3p^2 {}^2D_{3/2} \rightarrow 3s_3p_3d {}^2F_{5/2}^0$, where ${}^2F_{1/2}^0$ is an autoionizing level. Underhill has proposed that this broadening and the broadening of the emission observed in P Cygni at the same wavelength are due to a lowering of the ionization limit that turns the ${}^2D_{5/2}$ level into an autoionizing one. We have been able to verify that our results would not be affected by a lowering of the ionization limit.

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