NON-LTE LEVEL POPULATIONS OF SI II IN SUPERNOVA ENVELOPES

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Solutions of the statistical rate equations for a 15-level representation of Si II are compared with rough estimates.

INTRODUCTION

For many years, the spectra of supernovae have been little understood. However, recently a thermal model has gained acceptance in the interpretation of supernova spectra near maximum light. This model has spectral lines formed in a cooling, rapidly expanding envelope. The photosphere has been found to be expanding at a constant rate and this has led to a power law formulation for atomic and electron densities as a function of radius and time (1). With this model, line intensities can be estimated and the expected line, or absence thereof, can be sought in observed spectra.

Given the physical conditions in the envelope, local thermodynamic equilibrium conditions are not expected to hold, so that line intensities may not be calculated in the usual fashion. Instead, the statistical rate equations must be solved to find the level populations at each point in the envelope. Normally, this involves the simultaneous solution for the transfer of line radiation and therefore a large-scale iterative procedure. However, because of the rapid differential expansion of the envelope, line transfer may be treated by the escape probability method as developed by Sobolev (2) and Castor (3). Photons generated at a point are either reabsorbed locally or are Doppler-shifted out of resonance and then either strike the photosphere or escape completely. This allows the radiation field to be treated in a local fashion.

Rough estimates using the dominance of radiative over collisional rates suggest that ionization ratios should be given approximately by $N^*/N = W^2 N^{**} / N^* Eq. 1$

and level populations by

where N refers to the number density of the ion of interest, N⁺ is the number density of the next ionization stage, N_i is the number density of the ith level of the ion, 1 refers to the ground state, * refers to the LTE populations, and $W = 1/2 [1 - (1-R_0^2/r^2)^{1/2}]$ Eq. 3

is the geometric dilution factor for the radiation field. R_c is the photosphere radius and r is the radius of the point of interest in the envelope.

On the basis of arguments like these, some line identifications have been made. (See Oke and Searle (4) for a review of supernova spectra through 1973.) One prominent line in Type 1 supernovae has been attributed to $\lambda 6355$ line of Si II (1). This paper describes the complete calculation of the level populations of a 15-level representation of the Si II ion and compares the result with the rough estimates.

METHOD

In statistical equilibrium, which is assumed, the level populations of an ion are determined by the fact that the rate of transition into any level is equal to the rate out of that level. So, we write for level i

$$\sum_{i \neq i} N_j [C_{jk} + R_{jk}] + N_e N^{\dagger} \alpha_i + N_e^2 N^{\dagger} \gamma_i = N_i [\sum_{i \neq i} (C_{ij} + R_{ij}) + C_{ik} + R_{ik}] Eq. 4$$

 $N_{1}/N_{1} = W N_{1}^{*}/N_{1}^{*}$

Eq. 2

where N_e is the electron number density, C_{ij} and R_{ij} are the collisional and radiative bound-bound rates from level i to level j, γ_i and α_i are the collisional and radiative recombination coefficients, and C_{iK} and R_{iK} are the collisional and radiative ionization rates. The R_{ij} depend on the mean intensity of the radiation field in the transition. For a more detailed discussion of the application of the escape probability method to the treatment of this line radiation, see Castor and Van Blerkom (5). The rate equation for level i becomes

$$\sum_{u>i}^{l} \sum_{u < i}^{N_{u}(N_{e} c_{ui} + A_{ui} \beta_{ui} + B_{ui} M_{ui} I_{c}) + \frac{1}{k < i}} \sum_{x < i} \sum_{N_{z} (N_{e} c_{zi} + B_{zi} M_{z} I_{c}) + N_{e} N_{i}^{*} (a_{i} + N_{e} Y_{i}) = N_{i} \left\{ \sum_{u > i} [N_{e} c_{iu} + B_{iu} M_{B} I_{u} I_{c}] + \sum_{k < i} [N_{e} c_{i} + A_{iz} \beta_{ik} + B_{iz} M_{B} I_{z} I_{c}] + N_{e} c_{ix} + 4\pi \int_{v_{u}}^{\infty} a_{i} [v] \frac{J_{v}}{hv} [1 - exp(-hv/kT_{e})/b_{i}] dv \right\}$$
Eq. 5

where A_{ui} , B_{ui} and $B_{\ell i}$ are the Einstein coefficient of spontaneous and induced emission and absorption, $c_{ui} = C_{ui}/N_e$, I_c is the intensity of the core radiation, $a_i [\nu]$ is the photoionization cross-section af the ith level, ν_i is the threshold frequency, J_{ν} is the mean intensity of the continuous radiation field, T_e is the local electron temperature, b_i is the coefficient of deviation from LTE ($b_i = N_i/N_i^*$) and β_{ui} is the photon escape probability

$$\beta_{ui} = \beta_{iu} = [1 - exp(-\tau_{iu})]/\tau_{iu}$$
. Eq. 6

The line optical depth is

 $\tau_{iu} = \frac{\pi e^2}{mc} (gf)_{iu} [(N_i/g_i) - (N_u/g_u)]r \div [v_{ui}v(r)/c]$ Eq. 7

where g_i is the statistical weight of the ith level, f is the oscillator strength, v_{ui} is the frequency for the transition, and v (r) is the velocity of the envelope at radius r. We see that the escape probabilities depend on the (unknown) level populations in a nonlinear way. This means we must estimate the populations, calculate the escape probabilities, solve the rate equations for a new set of populations, and iterate until convergence is achieved.

The necessary atomic parameters were obtained as follows. Oscillator strengths were taken from Wiese *et al.*, (6) Curtis and Smith (7), Livingston *et al.* (8) and Kurucz and Peytremann (9). The Einstein coefficients were calculated from the oscillator strengths. Collisional excitation and de-excitation rates were calculated by the formulae given by Van Regemorter (10). Photoionization cross-sections were obtained from Allen (11) for the four given levels, the rest being calculated in the hydrogenic approximation. Radiative recombination rates were calculated from the formulae of Burgess and Seaton (12) and the three-body recombination coefficients were then calculated by detailed balancing.

The other necessary information deals with the conditions in the supernova envelope. The photosphere is assumed to radiate like a blackbody. The mean continuum intensity, J_{ν} , is treated in the same fashion as by Castor and Van Blerkom (5). The electron temperature is taken to be constant in the envelope, and equal to the temperature of the photosphere. The temperatures and electron densities at the photosphere as a function of time are summarized in Table 1. Since Type I supernovae are deficient in hydrogen (13) and perhaps also helium, conditions of solar abundance, no hydrogen and no hydrogen or helium are considered. The total density is taken to decrease outward as r^{-7} and to decrease with time as t^{-3} due to expansion. The velocity, which is proportional to radius, is taken to be 10,000 km/sec at the photosphere. The total amount of Si II and Si III was determined by applying Eq. 1 to the first four

ionization stages of Si.

The model chosen to represent the Si II atom is shown in Figure 1. This model should be sufficient for calculating the population of the 4s 2 S level, which controls the strength of the 6355 line, and may be adequate for the 3d 2 D level, which controls the strength of the λ 4130 line.

TABLE 1.	Supernova	envelope	parameters
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$\frac{\mathbf{t} - \mathbf{t}_0}{(\text{days})}$	T (K)	N _e (cm ⁻³)a solar xH xH,He		
-5	35000	1.7×10 ¹¹	3.4×10 ¹¹	2.6×1011
Ö	17000	$2.7 imes 10^{10}$	$2.7 imes 10^{10}$	$2.7 imes 10^{10}$
5	12000	$8.8 imes 10^{9}$	$8.8 imes10^9$	$6.0 imes 10^9$
10	9300	$3.9 imes 10^9$	$6.0 imes 10^{8}$	$2.2 imes 10^{9}$
15	7700	$2.0 imes 10^{9}$	$2.2 imes10^7$	$1.1 imes10^9$
20	6200	$9.0 imes 10^{8}$	$6.0 imes10^6$	$6.0 imes 10^8$
25	4900	$4.0 imes 10^{7}$	$2.3 imes 10^{6}$	$1.3 imes 10^{8}$

a See text for explanation

RESULTS

The results of the detailed calculations are compared with the rough estimates in Figure 2. For each level.

$$r_i = \log \left[(N_i/N_1) / (N_i^*/N_1^*) \right] / \log W$$
 Eq. 8

is plotted. P_i gives the dependence of the level population on the radiation field at $r = R_c$ for the case of no hydrogen or helium. Since the change in the values of P_i as a function of time differ somewhat depending on chemical composition, Figure 2 only shows the general trend. Also, for most levels, P_i is *not* a function of r. (Calculations were performed for $r/R_c = 1.0$ to 1.4 in increments of 0.1.) The few levels for which this is not true do not produce lines in the visible part of the spectrum. An x indicates the value of P_i at t = -5 days, where t is the time from maximum light. If P_i changes significantly with time, an arrow is drawn to the value at t = 25 days. If it does not, the single x indicates the average value. According to the rough estimate (Eq. 2), P_i should be unity for all levels at all times. Also in Figure 2,

$$P^{+} = \log \left[(N^{+}/N) / (N^{+*}/N^{*}) \right] / \log W$$
 Eq. 9

is shown in the column marked "ion". According to Eq. 1, P⁺ should be equal to two.

We see that at the earliest time, $P_i \simeq 1$ for all levels. This is an indication of the fact that, at these times, all levels are dominantly fed by one photoexcitation from the ground level. For example, level 6 $(4p^2P^0)$ is mainly populated by radiative decay from levels 8 (5s ²S) and 9 (4d ²D) which are populated by single photoexcitations from the ground. As time increases and the temperature drops, P_i increases for upper levels. This is an indication that as the ultraviolet flux decreases, the upper levels are no longer directly populated from the ground level, but rather by a multistep process, each depending on the dilution of the radiation field. P⁺ is about 1.7 for all values of t at $r = R_c$. This is because photoionization from the ground level is almost equal to the total photoionization from the other levels. For larger r, P⁺ increases to about 2 when the continuum optical depth becomes very large.



The approximations used here for collisional rates may not be very accurate for Si II. However, for most levels, collisional

DISCUSSION



FIGURE 2. P vs. level. The solid horizontal lines mark the rough estimate values from Eqs. 1 and 2. The other symbols are explained in the text.

FIGURE 1. The representation of Si II used in the calculations. The solid line indicates the $\lambda 6355$ transition and the dashed line indicates the $\lambda 4130$ transition.

rates were smaller than the radiative rates by many orders of magnitude. Only in transitions between levels 5 and 6 and levels 13, 14 and 15 did collisional excitation or de-excitation approach ten per cent of the photoexcitation or radiative de-excitation. In fact, C_{jk}/R_{ik} (see Eq. 4) is typically of order 10^{-4} to 10^{-5} . Collisional ionization and recombination rates were not important in any case. It should be emphasized that, since only the 4s ²S and, secondarily, the 3d ²D levels were of interest, the populations of the upper levels need not have been well determined.

These calculations validate the use of Eqs. 1 and 2 for use in calculating the level populations of Si II which are of interest. Currently, line strengths for many ions are being estimated (14) using the rough method. Future plans include detailed calculations for H and He I as a check on the estimates in those cases.

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