

CHARGE TRANSFER IN HELIUM-RICH SUPERNOVA PLASMA

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ABSTRACT

Charge transfer rate coefficients are estimated using Landau-Zener and modified Demkov approximations. The coefficients, augmented by those available from the literature, are used in statistical equilibrium equations describing the state of helium-rich supernova plasma. Such a plasma may describe both Type Ib and Type Ic supernova ejecta. The hypothesis that extensive mixing of metals with helium in Type Ic supernovae may provide a catalyst for rapid charge transfer that weakens the helium line emission by altering the excitation balance is tested. It is shown that charge transfer as a mechanism for suppressing helium line emission is ineffective unless the metal abundance is comparable to or larger than the helium abundance. This result supports an earlier conclusion that Type Ic supernovae must be helium poor relative to Type Ib events.

Subject headings: atomic data — atomic processes — plasmas — supernovae: general

1. INTRODUCTION

Type Ib and Type Ic supernovae have similar late-time ($t \gtrsim 100$ days) optical spectra (Wheeler & Harkness 1990; Harkness & Wheeler 1990; Filippenko 1991) and perhaps similar origins in helium-rich cores of massive stars that have lost their hydrogen envelopes prior to explosion (Shigeyama et al. 1990; Branch, Nomoto, & Filippenko 1991). These two classes are spectroscopically characterized near maximum light ($t \sim 1$ month) by the presence (Type Ib) or absence (Type Ic) of strong optical helium lines. Light curve models suggest Type Ib (Ensmann & Woosley 1988; Swartz & Wheeler 1991) are more massive than Type Ic events (Shigeyama et al. 1990; Nomoto, Filippenko, & Shigeyama 1990) though observationally there are exceptions to this trend (Wheeler & Harkness 1990; Baron 1992). Simulations of the explosion dynamics (Hachisu et al. 1991) conclude low-mass helium cores become more extensively mixed than high-mass cores.

Strong helium lines are expected when the helium regions of the ejecta are excited by products of radioactive ^{56}Ni and ^{56}Co decay (Harkness et al. 1987; Branch et al. 1991; Lucy 1991; Swartz et al. 1993). This can occur either by mixing the radioactive elements into the helium or by minimizing the ejecta mass so that the optical depth to γ -rays between the helium and the radioactive regions is low. As first anticipated by Branch et al. (1991), this implies the mixed, low-mass helium core model for Type Ic should have *stronger* helium lines than Type Ib in contradiction to spectroscopic observations. Based on model atmosphere spectra of the exploding helium stars of Shigeyama et al. (1990), Swartz et al. (1993) showed that this is indeed the case and concluded that Type Ic must therefore be helium poor while they supported the contention that these supernovae are low-mass, extensively mixed objects.

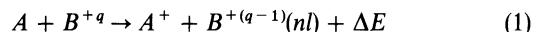
Mixing of the ejecta not only places radioactive material within helium-rich regions but also increases the metal content in these regions relative to helium. Metal enrichment increases the probability for rapid charge transfer reactions in general and for depletion of excited state populations of He I in particular. Can charge transfer processes alter the ionization-excitation structure in such a way as to weaken helium line

emission? If Type Ic are mixed and charge transfer significantly alters the helium ionization and excitation balance and charge transfer plays no role in unmixed Type Ib then these two classes of supernovae may both be helium rich and of similar evolutionary origin yet have distinctly different spectra.

This hypothesis is tested in the present study. The necessary charge transfer rate coefficients are calculated, to a reasonable approximation, in § 2. In § 3, statistical equilibrium equations are solved for “single-zone” representations of Type Ic supernova ejecta, based on the models of Swartz et al. (1993), to determine the effect of charge transfer on the ionization balance and on the helium excited state populations. There it is shown that charge transfer plays a minor role unless the helium/metal mass ratio is lower than about 0.4. Further discussion is given in § 4.

2. CHARGE TRANSFER RATES

Ion-atom charge transfer reactions of the form

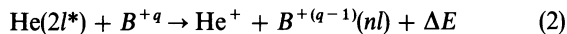


are possible in supernova plasma. Here, q is the initial charge on the ion, (nl) denotes an excited state, and ΔE is the asymptotic energy defect defined as the difference between the potentials of the quasi-molecular states formed by the entry and exit channels. That is, $\Delta E = I(B^{q-1}) - I(A) - E(nl)$ where I is the ionization potential and $E(nl)$ is the energy of the excited state. Ion-ion reactions are negligible at the low temperatures characteristic of SNe ($T_e \sim 5000$ K) because the Coulomb barrier present in the entrance channel prevents close encounters. The theories to be outlined below are applicable to two-state processes in which an electron bound to one reactant is transferred to an excited or ground state of the product (Bates 1960; Melius 1974). This restricts reactions 1 to single charge transfer and to products in which ion A^{+} is in the ground configuration. Multiple charge transfer is probably unimportant to the overall ionization balance in general (Tarter, Weisheit, & Dalgarno 1979) though at high temperatures some reactions, such as $\text{C}^{+4} + \text{He}$, do proceed through double charge transfer more rapidly than through single charge transfer (Crandall et al. 1976; Shipsey, Browne, & Olson 1977; Dalgarno 1978). In the present work, ions with charge exceeding $q = 1$ are rare and

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double charge transfer should always be negligible. Measurable cross sections for some reactions in which both products are in excited states or in which ion A^+ is excited and B^{q-1} is in its ground state have been made in the laboratory (e.g., Rutherford et al. 1971; 1972a, b; Rutherford & Vroom 1972; Turner-Smith, Green, & Webb 1973). At low energies, however, most reactions of this type are unlikely (Melius 1974). Reactions involving rearrangement of the ionic core (Butler & Dalgarno 1980, McCarroll, Valiron, & Opradolce 1983) are easily treated using the Landau-Zener approximation and we include such reactions here although they are not strictly two-state processes and the accuracy of the results are uncertain (McCarroll et al. 1983). Again these reactions are in general slow at low energies.

Equation (1) ignores situations in which states in the entry channel are excited states. This is valid in the coronal approximation wherein all excitations including recombinations are followed immediately by transitions toward the ground state. This is a sufficiently accurate assumption for most atoms in supernovae following the initial recombination phase. For the present study, however, reactions of the following form are also of interest:



where l^* represents either the singlet or triplet S or P state. Reactions of the form 2 are treated in this work.

All reactions either of the form 1 or 2 are further assumed to take place only through radial coupling between molecular states of the same symmetry and to obey the Wigner-Witmer conservation rules for L-S coupling (Herzberg 1950). In addition, the allowed range of energy defects, ΔE , lie in the approximate ranges 0.0 to 1.2 eV for $q = 1$ (e.g., Rapp & Francis 1962; Olson 1980) and 1.8 to 5.5 eV (corresponding to crossing distances lying between 5 and $15a_0$, see § 2.1) for $q > 1$ (e.g., Steigman 1975; Dalgarno & Butler 1978).

2.1. Landau-Zener Theory, $q > 1$

The Landau-Zener (LZ) approximation (Landau 1932; Zener 1932; Stueckelberg 1932) is of relatively general applicability to multiply-charge ion-atom reactions. It is based on an asymptotic description of the energy levels of the entry and exit channels and not on the details of the form of the molecular wavefunctions and potential energy curves formed in the collision process. It is therefore relatively easy to implement and has been widely employed in astrophysics. At large internuclear separations, R , the interaction in the entry channel is dominated by the dipole-induced attractive polarization potential, $H_{11}(R) \sim \alpha q^2 e^2 / 2R^4$, where α is the polarizability of the neutral component. For $q > 1$, the repulsive Coulomb potential, $H_{22} \sim (q-1)e^2/R$, dominates in the exit channel. Thus, if the reaction is exothermic, the two potential energy curves will cross (in the diabatic sense) at some separation R_x .

The Landau-Zener cross section for a relative collision energy E is

$$\sigma(E) = 2\pi p \int_0^{b_x} 2w(1-w)b db \quad (3)$$

where b is the impact parameter, b_x is the maximum impact parameter allowing the crossing point, R_x , to be reached, and p is the probability that the collision proceeds initially along the potential energy surface H_{11} . The reaction transition probability, $2w(1-w)$, where w is the probability that a transition

occurs during a single pass through R_x , is given by

$$w = \exp \left(- \frac{4\pi^2 H_{12}^2}{h v_r \Delta F} \bigg|_{R=R_x} \right). \quad (4)$$

Here, H_{12} is the interaction Hamiltonian coupling the diabatic potential energy curves, v_r is the radial component of the relative velocity of collision, and $\Delta F = |dH_{11}/dR - dH_{22}/dR|$ is the difference in slopes of the entry and exit channel potential curves. Using equation (4) and a judicious change of variables, the cross section, equation (3), can be written in closed form as

$$\sigma(E) = 4\pi R_x^2 (1 + \lambda) [E_3(\eta) - E_3(2\eta)], \quad (5)$$

where E_3 is the third exponential integral and η follows from the argument of the exponential in equation (4):

$$\eta = \frac{4\pi^2 H_{12}^2}{h v (1 + \lambda)^{1/2} \Delta F} \bigg|_{R=R_x}, \quad (6)$$

$\lambda = -H_{11}(R_x)/E$, $v^2 = 2E/\mu$, and μ is the reduced mass of the system.

It remains to estimate R_x , $H_{12}(R_x)$, the diabatic potentials and their derivatives, and λ . Choosing $H_{11}(\infty) = 0$ to set the energy scale and ignoring higher order or short range interaction terms so that H_{nn} is given reasonably by the above asymptotic forms leads to $H_{22}(R) = (q-1)e^2/R - \Delta E$. Noting that the polarization potential, H_{11} , is relatively flat at $R \gtrsim R_x$ and $H_{11}(R_x) = H_{22}(R_x)$ by definition, then $R_x \sim (q-1)e^2/\Delta E$ to a good approximation (Steigman 1975; Butler & Dalgarno 1980). By the same argument, $\lambda = -H_{11}(R_x)/E$ is small and can be neglected. Further, ΔF is easily evaluated using the same asymptotic forms of the potentials. For this purpose, dH_{11}/dR can be neglected relative to dH_{22}/dR . These approximations have been made in the spirit of the LZ approximation and can be compared to the method described by Butler & Dalgarno (1980). In the LZ approximation, the off-diagonal matrix elements, H_{12} , are related to the energy of separation of the corresponding adiabatic potential curves, ΔU , at the crossing point, R_x , by $\Delta U(R_x) = 2H_{12}(R_x)$. A powerful empirical expression for the energy separation in terms of the crossing point has developed as more rates have been established (Dalgarno 1954; Olson, Smith, & Bauer 1971; Butler & Dalgarno 1980). For reactions which do not alter the ionic core configuration

$$\Delta U(R_x) = 27.2 R_x^2 \exp(-\beta R_x) \quad (7)$$

(Butler & Dalgarno 1980). Here, $\beta^2 = 2I$, where I is the ionization potential of the atom in the entry channel in atomic units and $\Delta U(R_x)$ is in eV. Appropriate expressions for reactions leading to core configuration mixing are also given in Butler & Dalgarno (1980).

Assembling these expressions leads to a form of the cross section that depends implicitly only upon the collision energy E , the energy defect ΔE , the probability p , and the reduced mass μ . Equation (5) can be rewritten

$$\sigma(E) = 4\pi R_x^2 p [E_3(\eta) - E_3(2\eta)] \quad (8)$$

where now equation (6) becomes

$$\eta = \frac{\pi^2 \Delta U^2 R_x^2}{h(2E/\mu)^{1/2} (q-1)e^2}. \quad (9)$$

The corresponding charge transfer reaction rate coefficient is the product of the cross section and the relative velocity aver-

aged over a Maxwellian. For the numerical integration, the Gauss-Legendre quadrature method given by Bienstock (1983) is used with quadrature weights from Abramowitz & Stegun (1972) while the exponential integrals are evaluated using the Cody & Thatcher (1968) algorithm.

2.2. Olson-Demkov Theory, $q = 1$

For $q = 1$, the asymptotic potential energy curves for both the entry and exit channels are dominated by dipole interactions and are both "flat" over a large range of internuclear separations. A different type of reaction mechanism exists in this case if the asymptotic curves lie close together. In this case, charge transfer occurs not because of a curve crossing but because the coupling between the states is comparable in strength to the potential energy separation (Olson 1972, 1980). The basic collision mechanism was first described by Stuckelberg (1932). Demkov (1964) presented analytical forms for the cross sections in the case of charge transfer and Olson (1972) modified these expressions to include contributions from transitions occurring at impact parameters $b \gtrsim R_x$. A related, though independent, treatment of the processes involved, including some comparison to experiments, is given by Rapp & Francis (1962).

Since the transition occurs preferentially near a point, R_x , the cross section is again given by equation (3) where now, however, R_x is given by the solution to $2H_{12}(R_x) = |H_{11}(R) - H_{22}(R)|_{R=R_x}$. The potentials must include the dipole term, $H_{nn}(R) \sim H_{nn}(\infty) - \alpha_{nn}e^2/2R^4$, so that $H_{12}(R) \sim \Delta E - |\alpha_{11} - \alpha_{22}|e^2/2R^4$. A value for R_x is obtained by substitution of this expression into equation (7) [recall $\Delta U(R_x) = 2H_{12}(R_x)$] and solution by a simple bisection method. The expression for the transition probability is now

$$w = \left[1 + \exp \left(\frac{2\pi^2 \Delta U(R_x)}{h\beta v_r} \right) \right]^{-1} \quad (10)$$

(Demkov 1964) which leads to

$$\sigma(E) = \pi R_x^2 \int_1^\infty \frac{dx}{x^3} \left\{ \frac{4 \exp^{-\delta x}}{(1 + \exp^{-\delta x})^2} \right\} \quad (11)$$

(Olson 1972) where

$$\delta = \frac{\pi^2 \Delta U}{h\beta v} \bigg|_{R=R_x} \quad (12)$$

The same approximation is made in deriving equation (11) as was done above for equation (8) that $\lambda = -H_{11}(R_x)/E$ is small and can be neglected.

2.3. Results

The theory outlined above has been applied to calculate rate coefficients. The elements He, C, N, O, Ne, Na, Mg, Si, S, Ar, Ca, and Fe are considered with $q = 1$ and $q = 2$ giving 264 possible combinations in the entry channel for equation (1) and an additional 88 possible combinations for equation (2). This list was reduced by first eliminating those reactions without favorable channels based on the energy defect criterion. The list was further reduced by imposing the Wigner-Witmer rules ($\Delta L = 0$, $\Delta S = 0$; Herzberg 1950). Those reactions remaining with more than five favorable exit channels were all assigned a large rate coefficient ($k = 5 \times 10^{-9} \text{ cm}^3 \text{ s}^{-1}$) without further computation. This is probably reasonable and avoids additional uncertainties which may arise when the number of

favorable exit channels is large (Butler & Dalgarno 1980; Ovchinnikova 1973). For the remaining reactions, rates for each favorable channel were computed and added to the total for that reaction assuming the temperature $T_e = 5000 \text{ K}$ as is typical of supernova plasma after the recombination phase. Results are listed in Table 1 and Table 2. Additional rates taken from the literature are given in Table 3.

Atomic data needed for the calculations are from the following sources: The energy levels are from Moore (1971) and ionization potentials from Allen (1976). Ground state dipole polarizabilities are from Teachout & Pack (1971), Thorhallsen, Fisk, & Fraga (1968) and Dalgarno (1962); for $L = 0$ He I states from Victor, Dalgarno, & Taylor (1968) and for $L = 1$ He I states the scaling law of Olson & Smith (1973) was used. For other excited states the ground state polarizability was used. The probabilities p were taken as the ratio of the products of the statistical weights in the exit to the entry channels (Rapp & Francis 1962; Neufeld & Dalgarno 1987). For several favorable reactions, all levels within a term contribute as favorable channels. These were treated as a single channel ignoring the fine-structure. The term statistical weight is then used and the excitation energy is given by the weighted average of the level energies within the term. Several of the probabilities, p , therefore become larger than unity by this simplification.

Comparison of the computed rates to those available in the literature support the view that the approximations used here

TABLE 1

CHARGE EXCHANGE RATE COEFFICIENTS FOR REACTIONS OF THE FORM:
 $A + B^{+q} \rightarrow A^+ + B^{+(q-1)}(nl) + \Delta E$

Reaction	Rate ^a	Reaction	Rate ^a
N + C(+2)	1.4(+01)	O + C(+2)	3.7(-01)
Ne + C(+2)	7.7(+00)	Mg + C(+2)	4.5(-05)
Si + C(+2)	2.2(-01)	S + C(+2)	1.5(-01)
Fe + C(+2)	2.1(+00)	He + N(+2)	4.1(-01)
C + N(+2)	1.1(-01)	O + N(+2)	5.5(-01)
Ne + N(+2)	7.0(-02)	Na + N(+2)	5.0(+00)
Mg + N(+2)	2.6(+00)	Si + N(+2)	9.9(-01)
Ar + N(+2)	3.9(-04)	Ca + N(+2)	5.0(+00)
Fe + N(+2)	2.1(+00)	He + O(+2)	2.8(-05)
Na + O(+2)	5.0(+00)	Mg + O(+2)	5.0(+00)
Si + O(+2)	7.5(-02)	Ar + O(+2)	3.0(+00)
Ca + O(+2)	5.0(+00)	Fe + O(+2)	1.6(-01)
C + Ne(+2)	9.8(-03)	Na + Ne(+2)	5.0(+00)
Mg + Ne(+2)	5.0(+00)	Si + Ne(+2)	5.0(+00)
S + Ne(+2)	3.8(-01)	Ca + Ne(+2)	5.0(+00)
Fe + Ne(+2)	5.0(+00)	C + Na(+2)	1.3(-01)
Mg + Na(+2)	5.0(+00)	Si + Na(+2)	5.0(+00)
S + Na(+2)	3.6(-01)	Ca + Na(+2)	5.0(+00)
Fe + Na(+2)	5.0(+00)	Ca + Si(+1)	2.1(-05)
N + Si(+2)	1.2(-01)	O + Si(+2)	9.3(-01)
Na + Si(+2)	2.3(-01)	Mg + Si(+2)	2.3(-03)
Ca + Si(+2)	2.1(+00)	Fe + Si(+2)	7.4(+00)
C + S(+2)	1.1(-04)	Na + S(+2)	5.0(+00)
Mg + S(+2)	5.0(+00)	Si + S(+2)	4.2(-04)
Ca + S(+2)	5.0(+00)	Fe + S(+2)	6.9(-01)
He + Ar(+2)	2.2(-01)	C + Ar(+2)	5.0(-03)
Na + Ar(+2)	5.0(+00)	Mg + Ar(+2)	5.0(+00)
Si + Ar(+2)	5.0(+00)	S + Ar(+2)	4.6(-02)
Ca + Ar(+2)	5.0(+00)	Fe + Ar(+2)	5.0(+00)
Na + Ca(+2)	3.5(-04)	Mg + Ca(+2)	1.8(+00)
Si + Ca(+2)	4.2(-03)	Fe + Ca(+2)	1.7(-01)
Na + Fe(+1)	5.0(+00)	Ca + Fe(+1)	1.2(+01)
C + Fe(+2)	5.0(+00)	O + Fe(+2)	5.5(-01)
Na + Fe(+2)	5.0(+00)	Mg + Fe(+2)	5.0(+00)
Si + Fe(+2)	5.0(+00)	S + Fe(+2)	5.0(+00)
Ca + Fe(+2)	5.0(+00)		

^a In $10^{-9} \text{ cm}^3 \text{ s}^{-1}$ at $T_e = 5000 \text{ K}$, power of 10 in parentheses.

TABLE 2

CHARGE EXCHANGE RATE COEFFICIENTS FOR REACTIONS OF THE FORM:
 $\text{He}(2l^*) + B^{+q} \rightarrow \text{He}^+ + B^{+(q-1)}(nl) + \Delta E$

Reaction	Rate ^a	Reaction	Rate ^a
He(2 ¹ P) + C(+1)	1.0(+01)	He(2 ³ P) + C(+1)	7.4(-01)
He(2 ¹ S) + N(+1)	1.8(+01)	He(2 ¹ P) + N(+1)	1.8(+01)
He(2 ³ P) + N(+1)	4.6(+00)	He(2 ¹ S) + O(+1)	3.3(+01)
He(2 ¹ P) + O(+1)	1.9(+01)	He(2 ³ P) + O(+1)	5.7(+00)
He(2 ¹ S) + Ne(+1)	5.0(+01)	He(2 ³ S) + Ne(+1)	5.8(+00)
He(2 ³ P) + Ne(+1)	1.5(+00)	He(2 ¹ S) + Mg(+1)	1.1(+02)
He(2 ³ S) + Mg(+1)	1.9(+01)	He(2 ¹ P) + S(+1)	8.9(+00)
He(2 ³ P) + S(+1)	1.1(+00)	He(2 ¹ S) + Ar(+1)	1.5(+01)
He(2 ¹ P) + Ar(+1)	1.7(+01)	He(2 ³ P) + Ar(+1)	5.0(+00)
He(2 ¹ S) + Ca(+1)	6.6(+01)	He(2 ¹ P) + Ca(+1)	5.7(+01)
He(2 ³ P) + Ca(+1)	1.2(+01)	He(2 ¹ S) + Fe(+1)	5.0(+00)
He(2 ³ S) + Fe(+1)	5.0(+00)	He(2 ¹ P) + Fe(+1)	5.0(+00)
He(2 ³ P) + Fe(+1)	5.0(+00)	He(2 ¹ S) + C(+2)	2.0(+01)
He(2 ³ S) + C(+2)	3.7(-01)	He(2 ¹ P) + C(+2)	9.8(+00)
He(2 ³ P) + C(+2)	2.3(+00)	He(2 ¹ S) + N(+2)	5.0(+00)
He(2 ³ S) + N(+2)	5.0(+00)	He(2 ¹ P) + N(+2)	5.0(+00)
He(2 ³ P) + N(+2)	5.0(+00)	He(2 ¹ S) + O(+2)	5.0(+00)
He(2 ³ S) + O(+2)	5.0(+00)	He(2 ¹ P) + O(+2)	5.0(+00)
He(2 ³ P) + O(+2)	5.0(+00)	He(2 ¹ S) + Ne(+2)	5.0(+00)
He(2 ³ S) + Ne(+2)	5.0(+00)	He(2 ¹ P) + Ne(+2)	5.0(+00)
He(2 ³ P) + Ne(+2)	5.0(+00)	He(2 ¹ S) + Na(+2)	5.0(+00)
He(2 ³ S) + Na(+2)	5.0(+00)	He(2 ¹ P) + Na(+2)	5.0(+00)
He(2 ³ P) + Na(+2)	5.0(+00)	He(2 ¹ S) + Si(+2)	5.0(+00)
He(2 ³ S) + Si(+2)	9.3(+02)	He(2 ¹ P) + Si(+2)	5.0(+00)
He(2 ³ P) + Si(+2)	5.0(+00)	He(2 ¹ S) + S(+2)	5.0(+00)
He(2 ³ S) + S(+2)	5.0(+00)	He(2 ¹ P) + S(+2)	5.0(+00)
He(2 ³ P) + S(+2)	5.0(+00)	He(2 ¹ S) + Ar(+2)	5.0(+00)
He(2 ³ S) + Ar(+2)	5.0(+00)	He(2 ¹ P) + Ar(+2)	5.0(+00)
He(2 ³ P) + Ar(+2)	5.0(+00)	He(2 ¹ S) + Ca(+2)	6.2(-01)
He(2 ¹ S) + Fe(+2)	5.0(+00)	He(2 ³ S) + Fe(+2)	5.0(+00)
He(2 ¹ P) + Fe(+2)	5.0(+00)	He(2 ³ P) + Fe(+2)	5.0(+00)

^a In $10^{+9} \text{ cm}^3 \text{ s}^{-1}$ at $T_e = 5000 \text{ K}$, power of 10 in parentheses.

are accurate to no better than an order of magnitude (Bates 1960; Dalgarno & Butler 1978; Dalgarno 1982). The $\text{C}^{+2} + \text{He}$ reaction has no favorable energy channel. A rate of $k \sim 1.4 \times 10^{-12} \text{ cm}^3 \text{ s}^{-1}$ is given by Butler, Heil, & Dalgarno (1980) for reactions from the metastable $\text{C}^{+2} (2p^3 P^o)$ state. Butler & Dalgarno (1980) obtain a rate of 3.1×10^{-10} for the

reaction $\text{N}^{+2} + \text{He}$ using the LZ approximation. This is very similar to the rate of 4.2×10^{-10} computed here. The LZ approximation is known to give poor results for the $\text{O}^{+2} + \text{He}$ reaction (Butler & Dalgarno 1980; Dalgarno, Butler, & Heil 1980a; Butler, Heil, & Dalgarno 1984). The value of 2.8×10^{-14} computed here is much less than the quantal calculation result of 2.0×10^{-10} . Using the R_x and ΔU -values from quantal calculations of the potential energy surfaces (Dalgarno, Butler, & Heil 1980a) the present method gives more reasonable results, as expected (Butler & Dalgarno 1980). The $\text{Ne}^{+2} + \text{He}$ reaction does not have favorable channels, consistent with the results of Butler & Dalgarno (1980) and Dalgarno, Butler, & Heil (1980b). The present results give a rate coefficient of 2.2×10^{-10} for the $\text{Ar}^{+2} + \text{He}$ reaction which can be compared to the value 1.3×10^{-10} estimated by Butler & Dalgarno (1980) using the LZ approximation. Nikitin et al. (1990) measured a value of 4.4×10^{-11} at 300 K consistent with the calculations of Friedrich et al. (1986) for this reaction. Assuming the rate scales as $T^{1/2}$ (constant cross section) implies a rate of 1.8×10^{-10} at 5000 K for $\text{Ar}^{+2} + \text{He}$.

Other published results can be extrapolated for a rough comparison to the present calculations. Albritton (1978) claims the $\text{He}^+ + \text{Ar}$ reaction is slow ($k < 1.0 \times 10^{-13}$) at 300 K consistent with the lack of favorable channels found here. Rutherford et al. (1971, 1972a, b) and Rutherford & Vroom (1972) measured several reactions at energies as low as 2 eV ($\sim 20,000 \text{ K}$) and then extrapolated their results to lower temperatures. The present calculations found no favorable channels for any of these reactions. Those found by Rutherford and coworkers to have moderate or fast rates (Table 3) are all two-electron processes leaving the donor atom in an excited state. Such reactions were not considered in the present calculations. For inclusion in Table 3, the rates of Rutherford et al. were extrapolated to $T_e = 5000 \text{ K}$ assuming either a constant cross section or a Langevin behavior ($\sigma \sim v^{-1}$; e.g., Langevin 1905; Steigman 1975), depending on the trend of the Rutherford et al. results. A low rate was calculated here for $\text{N}^+ + \text{O}$ consistent with the higher energy results of Stebbings, Smith, Gilbody (1963).

TABLE 3
PUBLISHED CHARGE EXCHANGE RATE COEFFICIENTS

Reaction	Rate ^a	Reference	Reaction	Rate ^a	Reference
He + C(+3)	1.2(-02)	1	He + C(+4)	1.0(-05)	1
He + N(+2)	3.1(-01)	1	He + N(+3)	1.5(-01)	1
He + N(+4)	2.4(+00)	1	He + O(+2)	1.7(-01)	2
He + O(+3)	1.1(+00)	1	He + O(+4)	7.2(-01)	1
He + Ne(+2)	1.0(-05)	1	He + Ne(+4)	1.5(+00)	1
He + Mg(+3)	8.0(-01)	1	He + Mg(+4)	2.4(+00)	1
He + Si(+3)	5.6(-01)	1	He + Si(+4)	1.2(+00)	1
He + S(+3)	7.5(-01)	1	He + S(+4)	7.6(-04)	1
He + Ar(+2)	1.3(-01)	1	He + Ar(+3)	1.0(-05)	1
He + Ar(+4)	1.2(+00)	1	Mg + N(+1)	5.0(+00)	3
Ca + N(+1)	9.0(-01)	4	Fe + N(+1)	3.7(-01)	5
Ca + O(+1)	3.0(+00)	4	Fe + O(+1)	7.1(-01)	5
Si + He(+1)	3.3(+00)	6	Na + C(+1)	1.1(+00)	6
Mg + C(+1)	1.1(+00)	6	Si + C(+1)	2.1(+00)	6
S + C(+1)	2.5(+00)	6	Fe + C(+1)	2.6(+00)	6
Na + Mg(+1)	1.1(-02)	6	Na + Si(+1)	2.7(+00)	6
Mg + Si(+1)	2.9(+00)	6	Fe + Si(+1)	1.9(+00)	6
Na + S(+1)	2.6(-01)	6	Mg + S(+1)	2.8(-01)	6
Si + S(+1)	1.6(+00)	6	Fe + S(+1)	1.8(-01)	6
Na + Fe(+1)	1.0(-02)	6			

^a In $10^{+9} \text{ cm}^3 \text{ s}^{-1}$ at $T_e = 5000 \text{ K}$, power of 10 in parentheses.

REFERENCES.—(1) Butler & Dalgarno 1980; (2) Butler et al. 1984; (3) Rutherford et al. 1971; (4) Rutherford et al. 1972b; (5) Rutherford & Vroom 1972; (6) Prasad & Huntress 1980.

Several rate coefficients at low temperatures (relevant to molecular cloud conditions) are tabulated in Prasad & Huntress (1980). Some of these are originally from the work of Rutherford et al. and are discussed above. No reference is given by Prasad and Huntress for the remaining reactions relevant to the present study. Since their table has been treated with skepticism in the past (Péquignot & Aldrovandi 1986), their rates were re-computed here assuming they are either of the form of equation (1) or of the similar form but with the ion A^+ left in an excited state and B^{q-1} left in the ground state in the exit channel. Even with this relaxed selection criteria, the only reaction found to have favorable channels leading to a rapid rate was $\text{Fe} + \text{C}^+$. (There were more than five favorable channels for this reaction so the default value of 5×10^{-9} was adopted.) The Prasad & Huntress (1980) value for this rate is 2.9×10^{-9} assuming a Langevin cross section.

The only results available for reactions of the type represented by equation (2) are those of Neynaber & Tang (1983). They measured the reaction cross sections for $\text{Ne}^+ + \text{He}(2^3\text{S}) \rightarrow \text{Ne}(3s^3\text{P}) + \text{He}^+$. Their measured value, $\sigma \sim 2.0 \times 10^{-15} \text{ cm}^2$ at $T_e \sim 5000 \text{ K}$, is consistent with their calculated cross section obtained using the Demkov theory and assuming $J - J$ coupling [Hund's case(c)]. The value computed here for this reaction is $\sigma \sim 1.0 \times 10^{-14}$.

3. APPLICATIONS

The charge transfer rate coefficients given in Tables 1 and 2 are admittedly of limited accuracy, especially when considered individually. Those of Prasad & Huntress (1980) in Table 3 are highly uncertain. In light of this, it would be inappropriate to embark upon a full model atmosphere spectral calculation in the detail presented previously (Swartz et al. 1993) for helium-star models of Type Ic supernovae. The importance of charge transfer is determined instead by comparing the ionization balance and level populations for a typical supernova environment with and without charge transfer included in the statistical equilibrium equations. A large change in level populations, beyond that attributable to the uncertainty in the charge transfer atomic data, would signify an important contribution from charge transfer.

In this spirit of simple analysis, we take as a standard of reference the physical conditions at a representative point in the atmosphere of the mixed Type Ic model of Swartz et al. (1993) at 60 days past maximum. This time is within the epoch of maximum helium emission in the models and in the observations of the Type Ib SN 1984L (Harkness et al. 1987). The physical conditions for this "single-zone" model are listed in Table 4. The model is treated as in the full atmosphere model except for the effects of radiative transfer: Optically thin conditions are assumed for the continua while the lines are treated in the Sobolev escape probability formalism. Only the ionization structure is determined, the temperature of the gas is fixed at 5000 K which is within 10% of the full model results. Thus energy conservation is not imposed. The heating by radioactive ^{56}Co decay is included in order to determine rates of ionization by energetic electrons associated with the radioactive energy deposition. These rates are given in Swartz (1991) as are rate coefficients for dielectronic and radiative recombination, collisional ionization, and helium bound-bound processes. The resulting set of statistical equilibrium equations describing the metal ionization balance in the coronal approximation and the first 11 He I level populations along with the He II and He III populations were solved by linearization fol-

TABLE 4A
REFERENCE MODEL PROPERTIES

Element Name	Mass Fraction ^a	Number Density	Neutral Fraction	$q = 1^b$ Fraction	$q = 2$ Fraction
He	6.88(-01)	1.03(+09)	0.88103	0.11864	0.00033
He I(2s ³ S)	3.41(+03)
He I(2s ¹ S)	1.18(+02)
He I(2p ³ P)	8.16(+01)
He I(2p ¹ P)	3.14(+00)
He I(3s ³ S)	1.08(-03)
C	3.40(-02)	1.69(+07)	0.91414	0.08571	0.00015
N	1.00(-03)	4.27(+05)	0.94354	0.05608	0.00038
O	1.00(-01)	3.74(+07)	0.83477	0.16409	0.00114
Ne	1.70(-02)	5.08(+06)	0.79804	0.19812	0.00382
Na	4.00(-05)	1.08(+04)	0.78300	0.21700	0.00000
Mg	1.20(-02)	2.99(+06)	0.62667	0.36512	0.00818
Si	3.60(-03)	7.69(+05)	0.86549	0.13203	0.00246
S	2.20(-03)	4.11(+05)	0.74549	0.24833	0.00614
Ca	1.20(-03)	1.79(+05)	0.46565	0.51438	0.01980
Fe	1.40(-01)	1.61(+07)	0.51079	0.46279	0.02620

^a Power of 10 exponent in parentheses.

^b q is charge on the ion.

TABLE 4B
REFERENCE MODEL PARAMETERS

Parameter	Value
T_e (K)	5.0(+03)
ρ (g cm^{-3})	1.0(-14)
D_γ ($\text{ergs g}^{-1} \text{ s}^{-1}$)	1.3(+08)

lowing the basic algorithm of Swartz (1990). The fractional populations of the first three ionization stages for each element, in the absence of charge transfer, are also listed in Table 4. Doubly ionized states account for less than 2% of the elemental abundances and need not be considered further.

For illustration, a series of models was derived from the reference model of Table 4 in which the helium mass fraction was scaled from the fiducial value by a factor f ($0.02 \leq f \leq 1.00$) while maintaining the ratios of the metals. Thus, if X_m represents the mass fraction of some metal in the reference model, $f = 1$, it scales as

$$X_m(f) = X_m \left(\frac{1 - fX_{\text{He}}}{1 - X_{\text{He}}} \right), \quad (13)$$

where X_{He} is the fiducial helium mass fraction from Table 4. The resulting atomic and singly-charged ionic state populations, relative to their values in the absence of charge transfer reactions, are shown in Figures 1 and 2 against the scale factor, f . The first five neutral helium states are similarly presented in Figure 3.

Qualitatively, the curves in Figures 1–3 are nearly horizontal lines indicating the dependence on the helium abundance is weak (note the linear scale used in Fig. 3). The populations of certain metal ionization states are, however, changed by more than an order of magnitude by charge transfer. The effects are most clearly illustrated by the behavior of the ionization stage originally least populated. For example, for a reaction of the form of equation 1, if $N_A \ll N_{B^{q-1}}$, where N denotes a number density, then Figures 1–3 may show a large change in N_A while that for B^{q-1} and/or A^+ may be insignificant. This is because charge transfer is essentially a number conserving process in which individual charge transfer rate coefficients may be large

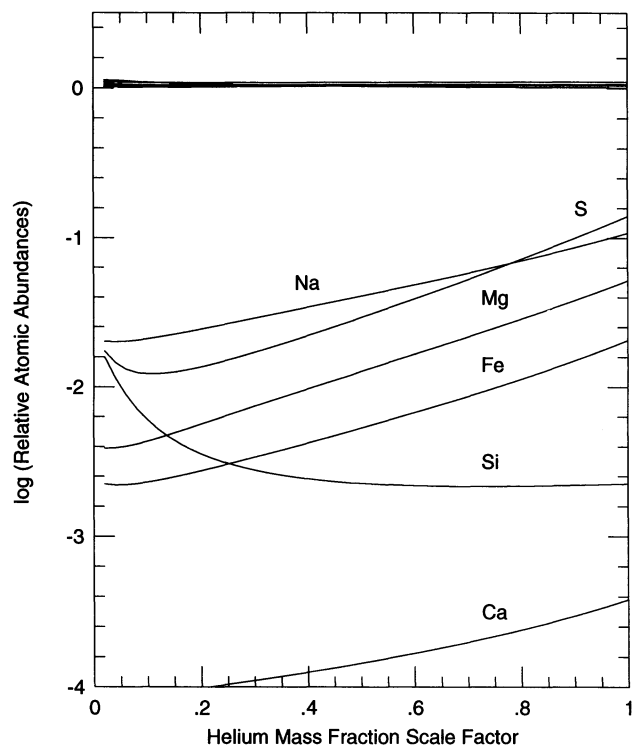


FIG. 1.—Logarithm of the ratio of the neutral state abundances including charge transfer in the rate equations to those computed without charge transfer is shown against the helium mass fraction scale factor, f . The total metal abundances scale as in eq. (13). The fractional distribution of the elements among their first three ionization stages is listed in Table 4 for the reference model ($f = 1$) in the absence of charge transfer.

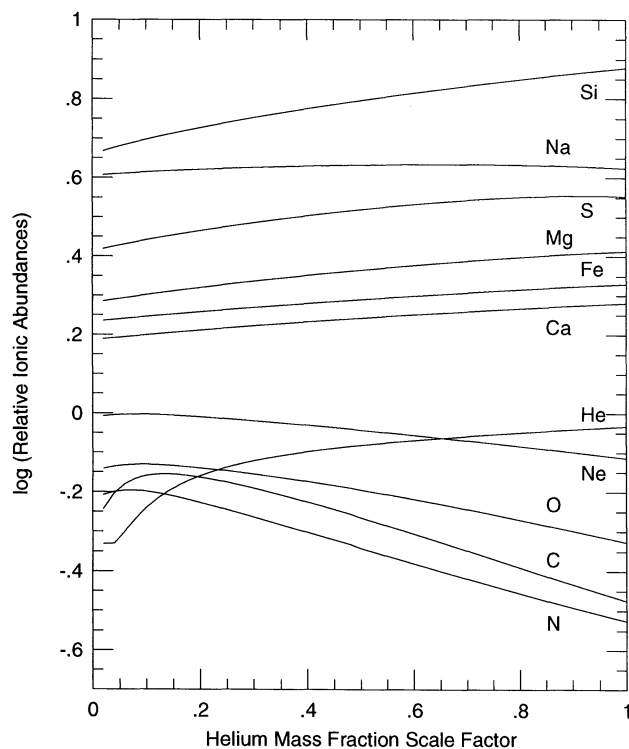


FIG. 2.—Relative ionized state abundances are shown as in Fig. 1

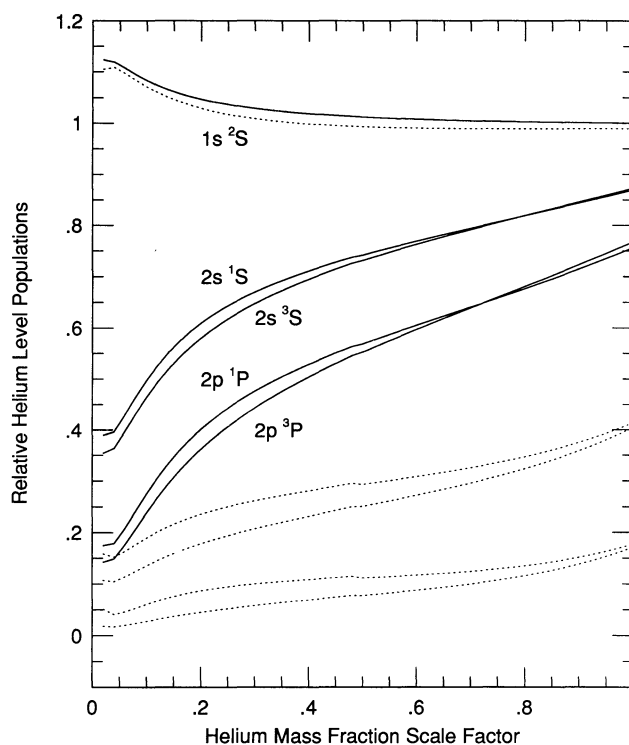


FIG. 3.—Ratio of the populations of the first five He I levels computed including charge transfer in the rate equations to those computed without charge transfer is shown (solid curves) against the helium mass fraction scale factor, f . The ratios for higher excited states (not shown) overlap with these first five levels. Charge transfer rates were not included for levels other than the first five. A factor of 2 change in the population of any level does not occur for helium mass fractions greater than $X_{\text{He}} \sim 0.3$ ($f \sim 0.4$). Such a small change suggests altering the helium excitation balance by charge transfer is ineffective in suppressing helium line emission. The dotted curves indicate the same ratio of the populations but using charge transfer rates 10 times larger than those listed in Tables 1 through 3.

though the effect may be small if the initial population of a reactant is large. This is the case for helium except at low values of the parameter f . It also accounts for the many abundance curves clustered about zero in Figure 1 but not in Figure 2. For other elements such as neon, there are no favorable rate coefficients so that the neon ionization balance is not affected by charge transfer even though its' total abundance is low.

Figure 1 illustrates the point that several metals undergo charge transfer ionization with other metals independent of the helium abundance. Tables 1 and 3 indicate most of the rates for these processes are those of Prasad & Huntress (1980). Even when the Prasad and Huntress rates are not included in the calculation, charge transfer still ionizes Fe, Ca, and Na. Neutral silicon is ionized primarily by reactions with helium. The impact of this on the helium level abundances is discussed below. It should be noted that the low-ionization elements Na, Mg, Ca, and Fe are preferentially photoionized to singly ionized states in supernova environments (Fransson & Chevalier 1989; Swartz et al. 1993). In a full model atmosphere calculation, it is doubtful that the effect of charge transfer on the neutral abundances of these elements would be as large as is suggested here. An exception to this may be iron. Based on a rather simplified atomic model for iron, Swartz et al. (1993) found that iron was photoionized to predominantly Fe^{+2} . In this case, charge transfer is certainly fast enough to recombine Fe^{+2} to form Fe^{+1} .

Figure 2 shows that almost all elements undergo some shift in their singly ionized state populations in the presence of charge transfer. The scatter of the curves is not large, however, with the maximum change less than an order of magnitude for any element. In particular, the relative He II abundance is unchanged except at low total helium abundance.

Charge transfer does not significantly affect the helium ionization balance nor the He I excited state level populations (Fig. 3). A factor of 2 or larger change in any level population does not occur for helium mass fractions exceeding 0.27. For the reference model, the maximum change in any level is less than 30%. Many of the rate coefficients ionizing helium from excited states are large (Table 2). The reason the overall effect is small is that the level populations are not driven by these rates but by (nonthermal electron impact) ionization from the ground state and (radiative) recombination toward excited states. These latter rates depend on the ground state and He II abundances which are many orders of magnitude larger than the excited state populations. In effect, there is an enormous reservoir of electrons available to fill the excited levels as they are depleted. Statistically, therefore, the level populations are unaffected by charge transfer. The variation with helium abundance exhibited in Figure 3 is due mainly to the helium charge transfer recombination reaction with Si I. As the total helium abundance becomes comparable to the silicon abundance, this reaction drives the ionization balance of helium which, in turn, influences the excited state populations by changing the partition of electrons between the He I ground state and He II "reservoirs." Without including the Si I + He II reaction in the rate equations, the He I level populations change by less than 20% independent of the helium abundance scale factor, f . There are no energetically favorable helium charge transfer reactions from the He I ground state.

As a crude test of the sensitivity to the tabulated rates, the rates were increased by an order of magnitude and the series of models repeated. Most of the atomic and ionic abundances are only weakly affected by this change. The largest changes were about a factor of 2. The He I excited state populations (Fig. 3) decreased by a factor of 2 to four for the reference model, $f = 1$, and by smaller factors for lower helium mass fractions. These are shown as dotted curves in Figure 3. These He I excited state populations represent an extreme upper limit to the effect of charge transfer in that rate coefficients an order of magnitude larger than those listed in Table 2 are physically unreasonable. Thus, overall, the results are not strongly sensitive to scaling the rates.

4. DISCUSSION

Charge transfer reactions dominate the ionization balance of many elements under many astrophysical conditions (Dalgarno & Butler 1978; Dalgarno 1982; Shields 1990). These include cool gas such as H I regions and molecular clouds (Péquignot & Aldrovandi 1986; Prasad & Huntress 1980) and the inter-stellar medium (Steigman 1975), as well as hotter environments such as quasars and X-ray photoionized nebulae (McCrack, Wright, & Hatchett 1977; Halpern & Grindlay 1980; Kallman & McCrack 1982; Shields 1990), and planetary nebulae (Péquignot, Aldrovandi, & Stasinska 1978; McCarroll et al. 1983). One condition all these cases have in common is an ionizing source that preferentially ionizes metals to multiply charged states while substantial amounts of hydrogen and helium remain neutral. In the cooler plasmas, the ionizing source is cosmic rays and, since the free electron abundance is low, charge transfer rates often exceed those for radiative

recombination by several orders of magnitude. In hotter environments, photoionization by hard photons removes the more tightly bound electrons leaving neutral hydrogen and helium relatively abundant. The high hydrogen and helium abundances coupled with high rate coefficients for $q \geq 2$ (e.g., Dalgarno 1982) ensure that charge transfer dominates radiative recombination for many metals while the hydrogen and helium ionization balance is hardly perturbed.

Supernovae, in contrast, are ionized by high-energy (MeV) electrons and positrons associated with radioactive decay. This source maintains a moderate degree of ionization (ionization fraction $X_e \sim 0.1$, higher for thermonuclear Type Ia explosions) for a considerable time ($t \gtrsim 1$ year) at rather low temperatures ($T_e \sim 5000$ K). Ionization by energetic electrons is only weakly dependent on the ionization potential of the target ion. As a consequence, the ionization balance is to zeroth-order independent of the ionization potential of the constituent elements in the plasma and most elements are predominantly distributed among neutral and singly ionized states (Table 4; Kosma & Fransson 1992). Relatively few favorable charge transfer channels exist in such an environment because charge transfer with singly charged reactants occurs over a much more restricted range of energy defects than with multiply charged reactants. As a result, transfer does not dominate the ionization balance of as many elements in supernovae as it does in other astrophysical environments.

The objective of the present work is to determine the influence of charge transfer on the ionization and excitation balance of helium in helium-rich Type Ic supernova models. The large helium abundance prevents charge transfer from altering the helium ionization and excitation balance. This is precisely the same effect found for hydrogen (and helium) in the many other astrophysical environments in which charge transfer has been studied: Charge transfer reactions may drive the ionization balance of the minor constituents but only weakly perturbs that of the dominant element. If the helium abundance is decreased relative to the metals then charge transfer tends to decrease the He I excited state level populations relative to their values in the absence of charge transfer. Swartz et al. (1993) roughly estimated that if the helium abundance is reduced to about 10% by mass then the hydrodynamic models of Shigeyama et al. (1990) may reproduce the observed optical spectra of Type Ic supernovae. The present work cannot improve upon that estimate because of the uncertainty in the charge transfer rates. It is reasonably certain, on the other hand, that charge transfer is ineffective for high helium abundances. Therefore, the helium abundance cannot be large in Type Ic supernovae.

Unfortunately, virtually nothing can be stated about the accuracy of the charge transfer rate coefficients estimated in this work. To do so requires a case by case comparison to rates derived by more elaborate means. The rates tabulated here should be plausible estimates of actual rates in many cases but should be used in the spirit of the present work, namely, to help identify the general trend of the effects of charge transfer on the overall ionization equilibrium. For this purpose, the rates can be assumed constant or to vary as $T^{1/2}$ within ~ 2 eV of the temperature used here (see also Butler & Dalgarno 1980 and the scaling law proposed by Arnaud & Rothenflug 1985).

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