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DIELECTRONIC RECOMBINATION: AN OVERVIEW OF THEORY AND EXPERIMENT, AND SOME ASTROPHYSICAL IMPLICATIONS

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RESUMEN

Se discute el estado actual de las tasas de recombinación dielectrónica (DR) usadas para modelar plasmas cósmicos. Se da una breve revisión de los estudios teóricos y experimentales sobre DR. Se muestran resultados que ilustran la relevancia astrofísica de las tasas de DR en estudios del medio intergaláctico.

ABSTRACT

The status of dielectronic recombination (DR) rate coefficients used for modeling cosmic plasmas is discussed. A brief overview of theoretical and experimental studies of DR is given. Results are shown which demonstrate the astrophysical importance of accurate DR rates for studies of the intergalactic medium.

Key Words: **ATOMIC PROCESSES — INTERGALACTIC MEDIUM — METHODS: ANALYTICAL — METHODS: LABORATORY**

1. INTRODUCTION

Dielectronic recombination (DR) is a two step recombination process which begins when an electron collisionally excites an ion and is simultaneously captured. The total energy of the recombined ion is in the continuum and it can autoionize. The DR process is complete when the recombined ion emits a photon which reduces the total energy of the system to below the ionization threshold for the recombined ion. The DR process in C IV can be expressed as

$$\mathrm{C}^{3+}(2s) + e^- \leftrightarrow \mathrm{C}^{2+}(2pnl) \quad \rightarrow \begin{cases} \mathrm{C}^{2+}(2snl) + h\nu \\ \mathrm{C}^{2+}(2pn'l') + h\nu. \end{cases} \tag{1}$$

Energy conservation requires that the incident electron kinetic energy E_k plus the binding energy E_b released in the capture must equal the energy ΔE needed to cause the core excitation (here the $2s-2p$ transition). Because ΔE and E_b are quantized, E_k is also quantized making DR is a resonant process. In general, low temperature DR occurs for plasmas where $k_BT_e << \Delta E$ and high temperature DR for $k_BT_e \sim \Delta E$. Excitation of the core electron can involve a $\Delta n = 0$ transition as shown above or a $\Delta n \geq 1$ excitation.

The core excitation and resulting radiative decay in the DR process can also be produced by electron impact excitation (EIE) of the initial ion. However, in DR the captured electron can screen the core and shift the energy of the emitted photon slightly from the EIE-produced photon. This creates satellite lines to the corresponding EIE-produced line. For capture into low-n Rydberg levels, this screening can be significant and the resulting line resolved from the EIE-produced line. For capture into high enough n levels, the screening of the core is insignificant and the satellite line cannot be resolved from the EIE line.

DR plays an important role in astrophysics because it is the dominant electron-ion recombination process for most ions in low density, photoionized and electron-ionized cosmic plasmas (Arnaud & Rothenflug 1985; Arnaud & Raymond 1992; Kallman et al. 1996). Accurate DR rate coefficients are needed to calculate reliably the ionization balance, thermal structure, and line emission of cosmic plasmas. Almost all DR rates currently used in astrophysics come from theoretical calculations. Compilations of recommended DR rates have been given by Shull & van Steenberg (1982), Arnaud & Rothenflug (1985), Arnaud & Raymond (1992), Ferland et al. (1998), and Mazzotta et al. (1998).

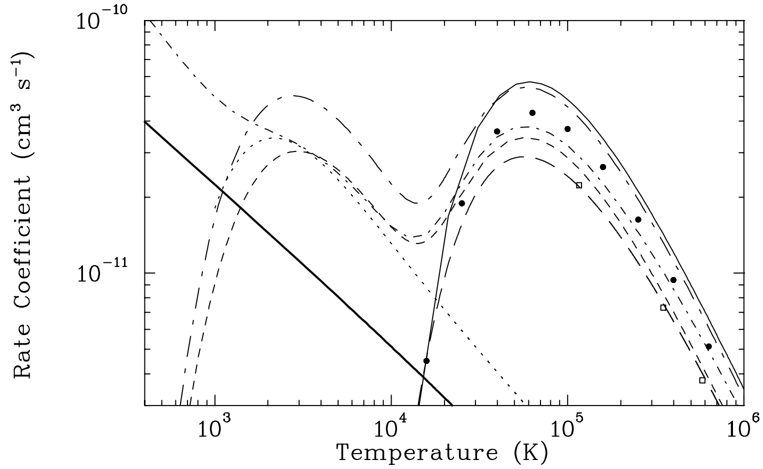

Fig. 1. Theoretical C IV to C III $\Delta n = 0$ DR rate versus electron temperature. Calculations are from Burgess (1965, thin solid line), Shull & van Steenberg (1982, long-dashed curve); Nussbaumer & Storey (1983, short-dashed curve); McLaughlin & Hahn (1983, medium-dashed curve); Romanik (1988, dotted-long-dashed curve); Badnell (1989, filled circles); Chen (1991, open squares); and Nahar & Pradhan (1997, dotted-medium-dashed curve), who calculated a combined RR+DR rate. The thick solid curve is the RR rate of Péquignot et al. (1991).

2. THEORETICAL RATE COEFFICIENTS

Accurate DR calculations are theoretically challenging. An infinite number of states can contribute to the DR process. Theoretical and computational approximations must be made to make the calculations tractable. An example of the difficulty of producing accurate DR rates is shown in Figure 1 which presents the published rates for $\Delta n = 0$ DR onto C IV.

The oldest DR rate in Figure 1 is that derived from the semi-empirical Burgess (1965) formula. This formula was designed to provide high temperature DR rates and not surprisingly does not produce the correct low temperature behavior. Here, at high temperatures the Burgess formula lies at the upper limit for the range of theoretical DR rates. In Fe XIX, Savin et al. (1999) found that the Burgess rate provided the lower limit for the theoretical DR rates. We infer from these comparisons that it is not possible to know a priori if the Burgess rate will lie at the lower or upper limit of the theoretical DR rates (or maybe somewhere in between).

There are a number of single-configuration, pure LS-coupling calculations shown in Figure 1. The rate of Shull & van Steenberg (1982) is derived from calculation of Jacobs, Davis, & Rogerson (1978) which does not account for low temperature DR. The rate of Nussbaumer & Story (1983) was calculated to provide the low temperature DR rate needed for modeling photoionized plasmas. Also shown in Figure 1 are the rates of McLaughlin & Hahn (1983) and Romanik (1988). There is a factor of ~ 2 scatter between these various LS-coupling calculations.

Pure LS-coupling calculations do not include all possible autoionization levels which contribute to the DR process. For lithiumlike ions such as C IV, LS-coupling accounts for only two-thirds of all possible autoionizing levels (Griffin, Pindzola, & Bottcher 1985). Taking this into account, one should multiply all of the LS-coupling calculations in Figure 1 by a factor of 1.5. For boronlike C II, N III, and O IV, including levels which are forbidden to autoionize in LS-coupling increases the DR rates by a factor of 1.7 at $T_e = 10^4$ K (Badnell 1988). Because of these missed autoionizing levels, LS-coupling calculations provide only a lower limit to the theoretical DR rate.

State-of-the-art DR calculations are carried out using multiconfiguration techniques. Figure 1 shows the multiconfiguration Breit Pauli (MCBP) calculations of Badnell (1989) which were carried out in intermediate coupling. The fully-relativistic, multiconfiguration Dirac-Fock (MCDF) calculations of Chen (1991) are also shown. Both the MCBP and MCDF calculations account for levels which are forbidden to autoionized in LS-coupling. These two calculations were carried out for high temperature plasmas and hence do not produce the correct low temperature behavior. There is a factor of ~ 1.5 difference between these two calculations.

Another state-of-the-art calculation shown in Figure 1 is the rate of Nahar & Pradhan (1997). They calculate a unified radiative recombination (RR) and DR rate for capture into levels $n \leq 10$ and use quantum defect theory to calculate the DR rate due to capture into levels $n > 10$. Unfortunately, their work is carried out in LS-coupling. Thus, the DR portion of their rate should probably be multiplied by a factor of 1.5. Taking this into account produces, at high temperatures, a factor of ~ 2 difference between their results and those of Chen (1991). Also, it is unclear what the source is of the discrepancy at $T_e = 400$ K between the recombination rate of Nahar & Pradhan and the RR rate of Péquignot, Petitjean, & Boisson (1991). At these temperature there are no DR resonances which contribute to the recombination process (Mannervik et al. 1998).

The lack of reliable DR rates is a major problem for modeling cosmic plasmas. Critical evaluations for DR rates onto ions with partially filled L and M shells suggests that there is a factor of ~ 2 uncertainty inherent in the different theoretical techniques used to calculate DR (Arnaud & Raymond 1992; Savin et al. 1997, 1999; Schippers et al. 1998). Low temperature rates do not exist for most third row and higher elements (Ferland et al. 1998). For many ions, only Burgess formula rates exist (Mazzotta et al. 1998). For others, single-configuration, pure LS-coupling calculations exist, but no state-of-the-art calculations exist. And even if such calculations did exist, their reliability in the absence of benchmark measurements is still questionable.

Some confusion as to the state of DR theory has been sown by the claim of Nahar & Pradhan (1997) that their recombination rates are accurate to 10–20%. This claim applies primarily to their non-LS coupling calculations for DR onto hydrogenic and heliumlike ions where radiation damping has been included. It does not apply to the majority of their work which has been carried out in LS-coupling without radiation damping.

The situation for DR rates onto hydrogenic and heliumlike ions is thought to be good. Where measurements and state-of-the-art calculations exist, the agreement is typically better than 20% (e.g., Beiersdorfer et al. 1992a; Müller 1995; Nahar & Pradhan 1997; Savin 1999). Unbenchmarked state-of-the-art DR theory is believed to produce reliable rates for DR onto these isoelectronic systems. The problem is that few state-of-the-art calculations exist for these systems.

3. LABORATORY MEASUREMENTS

State-of-the-art techniques for measuring DR involve using electron beam ion traps (EBITs; Levine et al. 1988; Beiersdorfer et al. this volume) or heavy-ion storage rings (Müller & Wolf 1997). EBIT measurements of DR detect the stabilizing photon in the recombination process. Storage ring measurements detect the recombined ions. EBIT and storage ring experiments can measure DR resonance strengths to accuracies of $\lesssim 20\%$.

Measurements have been carried out for ions of a number of cosmically abundant elements (i.e., with atomic number ≤ 30). These include measurements of DR onto hydrogenic He II (DeWitt et al. 1995 and references therein), C VI (Wolf et al. 1991), and O VIII (Kilgus et al. 1990); heliumlike C V (Kilgus et al. 1993; Mannervik et al. 1997), Ar XVII (Smith et al. 1996), and Fe XXV (Beiersdorfer et al. 1992a, 1992b); lithiumlike C IV (Mannervik et al. 1998; Müller et al. 1998), Ne VIII (Zong et al. 1998), Si XII (Kenntner et al. 1995; Bartsch et al. 1997), Ar XVI (Schennach et al. 1994), and Fe XXIV (Gu et al. 1999); boronlike Ar XIV (DeWitt et al. 1996); oxygenlike Fe XIX (Savin et al. 1999); fluorinelike Fe XVIII (Savin et al. 1997, 1999); argonlike Ti V (Schippers et al. 1998); and sodiumlike Fe XVI (Linkemann et al. 1995). Unfortunately most of these results have not been used to produce rate coefficients for modeling cosmic plasmas

In general, agreement between experiment and state-of-the-art theory has been good, though sometimes only after a couple of iterations of the theoretical calculations. Initial MCBP calculations for DR onto Fe XVI were a factor of ~ 2 larger than experiment. This discrepancy was later resolved by including more configurations in the calculations (Gorczyca & Badnell 1996). Measurements of DR onto Fe XVIII demonstrated the importance at low temperatures of DR via the $2p_{1/2} \rightarrow 2p_{3/2}$ electric-dipole-forbidden core excitation (Savin et al. 1997; 1999). This channel had not been included in earlier MCDF calculations which were primarily carried out for modeling high temperature plasmas (Chen 1988). Lastly, for some systems theory is still discrepant with experiment. For example, for DR onto Ar V, theory has not yet been able to reproduce the complicated low energy resonance structure which dominates the DR rate at low temperatures.

The history of comparisons between theory and experiment suggests that for DR onto L- and M-shell ions, theory cannot be benchmarked against a single ion in an isoelectronic sequence and then used reliably to

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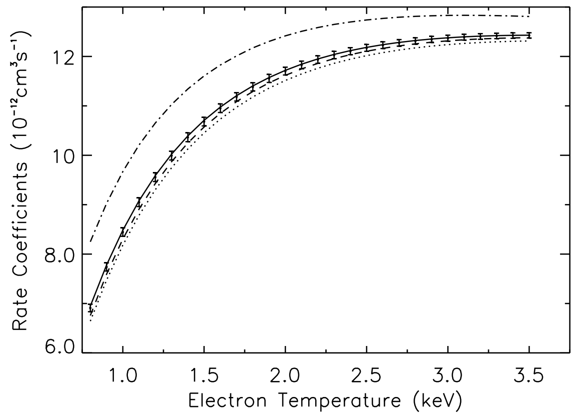

Fig. 2. Adapted from Gu et al. (1999). The rate coefficient for producing $3d_{5/2} \rightarrow 2p_{3/2}$ line emission due to EIE of and DR onto Fe XXIV. The error bars show the experimentally derived EIE rate coefficient. The dotted, dashed, and solid curves represent different theoretical EIE rates which are discussed in detail in Gu et al. The dashed-dotted curve shows the rate coefficient for $3d_{5/2} \rightarrow 2p_{3/2}$ line emission when DR satellite contributions, due to capture into $n \geq 5$, are included.

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produce DR rates for all other ions in the sequence. There is good agreement between state-of-the-art theory and experiment for DR onto K-shell ions, and theory is believed to be able to produce reliable DR rates for those K-shell ions where no measurements exist.

In the rest of this section, we present some recent EBIT and storage ring results which are of particular interest for modeling cosmic plasmas.

3.1. *Line Emission*

As mentioned in Section 1, DR can be an important line emission mechanism in cosmic plasmas. In heliumlike ions, the ratio of DR-generated to EIE-generated lines is a well known temperature diagnostic (Dubau & Volonté 1980). For the DR produced lines, the relevant K-shell emission has been reasonably well studied experimentally (e.g., Beiersdorfer et al. 1992a; Wargelin 1993).

In the past less attention has been paid to DR-generated line emission in L-shell ions. This has changed with the recent launching of *Chandra* and the upcoming launches of *XMM* and *Astro-E*. The spectrometers onboard these satellites are designed to resolve the L-shell emission in iron. Analyzing the collected spectra will require not just accurate EIE rates for producing the observed lines but also accurate rates for the DR satellites which blend with the EIE lines.

Recently Gu et al. (1999) initiated a series of EBIT experiments to measured DR contributions to iron L-shell line emission. In their first paper they present results for DR onto Fe XXIV producing X-ray satellite lines which blend with EIE lines in Fe XXIV. An example of their results is shown in Figure 2 which shows the experimentally derived rate for producing $3d_{5/2} \rightarrow 2p_{3/2}$ line emission due to EIE of and DR onto Fe XXIV. At temperatures where Fe XXIV is abundant, unresolved DR satellites contribute $\sim 10\%$ to the total line emission. Including contributions due to DR into levels $n < 5$ is estimated to make the DR contribution $\sim 20\%$.

The results of Gu et al. (1999) also demonstrate the importance of DR satellites for lines whose lower level is not the ground level. Commonly used spectral codes such as MEKAL (Mewe, Kaastra, & Liedahl 1995) do not include these DR satellite contributions for most L-shell iron ions. Gu et al. showed that the DR satellite contribution to $3d_{5/2} \rightarrow 2p_{3/2}$ line emission is equally, if not more, important that the DR contributions to the $3p_{3/2} \rightarrow 2s_{1/2}$ and $3p_{1/2} \rightarrow 2s_{1/2}$ line emission. This was first predicted theoretically by Zhdanov (1982).

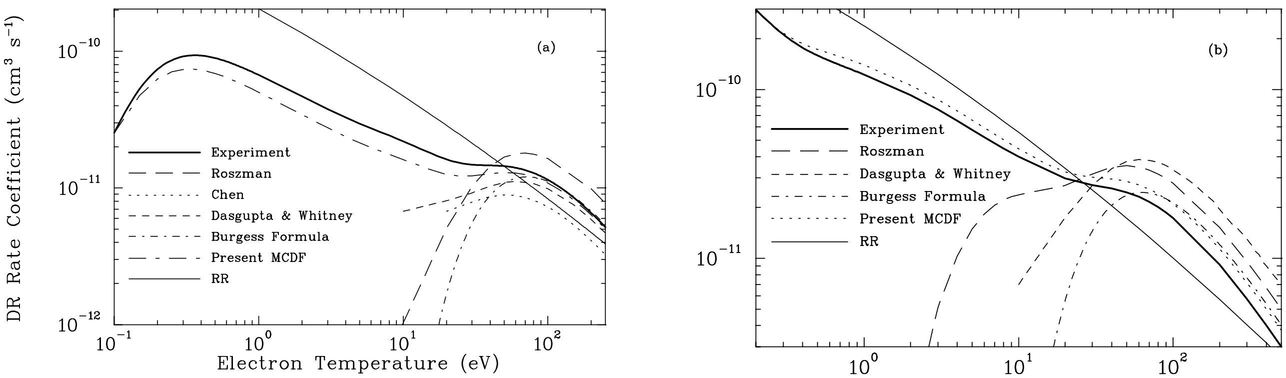

Fig. 3. From Savin et al. (1997, 1999). Low temperature DR rates (here $\Delta n = 0$) for *(a)* Fe XVIII to Fe XVII and *(b)* Fe XIX to Fe XVIII. The thick solid curve shows the experimentally derived rates. The dotted-long-dashed curve in *(a)* and the dotted curve in *(b)* show the new MCDF calculations of Savin et al. The thin solid curve shows the recommended RR rate of Arnaud & Raymond (1992). The other curves show DR rates published before the measurements were carried out. See Savin et al. for more details.

3.2. *Rate Coefficients for X-Ray Photoionized Plasmas*

Iron ions play an important role in determining the thermal stability of X-ray photoionized plasmas which form in the media surrounding active galactic nuclei (AGN) and X-ray binaries (XRBs; Hess, Kahn, & Paerels 1997). Recent *ASCA* observations of the XRB Cyg X-3 have detected line emission from ions predicted to form in regions where the gas is believed to be thermally unstable (Liedahl & Paerels 1996). This raises many questions, one of which is the accuracy of the atomic data used to model photoionized plasmas. Of particular concern is the accuracy of the relevant low temperature DR rates for the iron L-shell ions.

Recently Savin et al. (1997, 1999) have initiated a series of storage ring measurements to produce reliable low temperature DR rates for the iron L-shell ions. Their results for DR onto Fe XVIII and Fe XIX are shown in Figure 3. Fe XVIII and Fe XIX are predicted to peak in abundance at temperatures of ~ 20 eV and 40 eV, respectively, in photoionized gas with cosmic abundances (Kallman et al. 1996). At these temperatures there is a factor of 2 to order of magnitude scatter among those theoretical calculations published before the measurements were carried out. The experimentally derived DR rates are estimated to be accurate to better than 20%. New MCDF and MCBP calculations agree with the experimentally derived rates to within $\lesssim 35\%$.

Of particular note is the importance of DR via $2p_{1/2} \rightarrow 2p_{3/2}$ core excitations. These channels are important only at low temperatures. Most DR calculations in the literature have been carried out for modeling high temperature plasmas and have not accounted for these channels. Savin et al. (1997) showed that for Fe XVIII this is the dominant DR channel in photoionized plasmas. Line emission due to DR via these fine-structure channels also offer the possibility of new electron temperature and density diagnostics (Savin et al. 1998).

Based on their results, Savin et al. (1999) estimate there is a factor of 2 uncertainty in the published iron L-shell $\Delta n = 0$ DR rates. They have investigated the effect this uncertainty has on the predicted thermal stability of X-ray photoionized gas. They find that while the uncertainty cannot remove the thermal instability, it does dramatically affect the range in parameter space over which the instability exists.

3.3. *Field Effects*

Electric and magnetic fields have been detected or inferred for many different cosmic plasmas. Electric fields of ~ 10 V cm^{-1} have been estimated for the solar transition region (Reisenfeld 1992). Fields of ~ 170 V cm^{-1} have been inferred for coronal loops (Foukal, Hoyt, & Gilliam 1983). Magnetic fields of 10–45 G have been detected in the solar transition region (Mariska 1992). Fields of up to 1500 G have been inferred in stellar photospheres (Donati et al. 1997) and coronae (Brickhouse & Dupree 1998). AGN have estimated fields of $10^4 - 10^5$ G (Celotti, Fabian, & Rees 1992). And white dwarfs have estimated fields of 0.01–1000 MG (Schmidt 1987).

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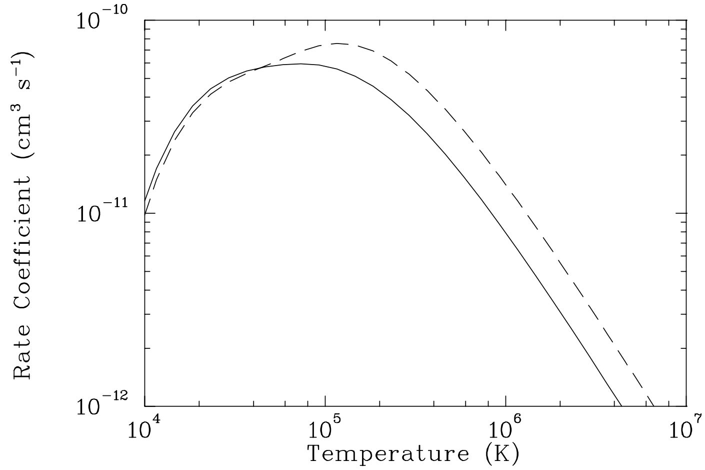

Fig. 4. Adapted from Bartsch (1999). $\Delta n = 0$ DR onto Si XII for $E \sim 0$ V cm^{-1}, $B \sim 0$ G (solid curve) and for $E = 181$ V cm^{-1}, $B = 418$ G (dashed curve).

Electric fields have been predicted to enhance the DR process (Jacobs et al. 1976). This was confirmed by laboratory measurements (Müller et al. 1986; Savin et al. 1996). In these experiments the ions travel through an applied magnetic field, creating a Lorentz electric field perpendicular to the magnetic field. The first storage ring measurements of field enhanced DR were carried out in Si XII by Bartsch et al. (1997). The results were discrepant with calculations carried out for a purely electric external field. Robicheaux & Pindzola (1997) proposed that it is not just the electric field, but also the perpendicular magnetic field which affects the DR process. This has since been confirmed by further experiments (Bartsch et al. 1999; Klimenko, Ko, & Gallagher 1999).

In Figure 4 we show the $\Delta n = 0$ DR rate for recombination onto Si XII for two different sets of external fields (Bartsch 1999). Measurements were carried out for capture into Rydberg levels $n \lesssim 50$ and do not include contributions from $n \gtrsim 50$ levels. DR into these high n levels is readily enhanced by external fields, so the field enhancement shown in Figure 4 represents only a lower limit. Si XII is predicted to form in photoionized gas of cosmic abundances at $k_B T_e \sim 2 \times 10^5$ K. At these temperatures, the fields used by Bartsch enhance the DR rate by a factor of ~ 1.6. The fields used by Bartsch are not that different from those expected in cosmic plasmas. For instance, thermal motion through estimated AGN magnetic fields of $10^4 - 10^5$ G produces electric fields of $\sim 80 - 800$ V cm^{-1}.

4. ASTROPHYSICAL IMPLICATIONS

The uncertainties in the DR rates used for modeling cosmics plasmas affect many different astrophysical issues. For extragalactic H II regions, these uncertainties affect the inferred primordial He abundance (Ali et al. 1991). For AGN and XRBs, uncertainties in the low temperature DR rates for the iron L-shell ions affect the thermal structure of the X-ray photoionized gas and can dramatically alter the range in parameter space over which the well-known thermal instability of the gas exists (Savin et al. 1999). In stellar atmospheres, uncertainties in the iron DR rates can change the predicted emission measure distribution by an order of magnitude. This has important implications for the heating and cooling of stellar coronae (Brickhouse 1996). And in solar observations, uncertainties in DR rates introduce factors of ~ 2 errors in derived abundances and hinders studies of the FIP effect in the solar corona (Doschek et al. 1998).

4.1. *The Intergalactic Medium*

Recently, Savin (2000) has investigated the effects of the uncertainties in DR on the ionization structure of the intergalactic medium (IGM). The hydrodynamic, cosmological simulations of Hellsten et al. (1998) and the plasma modeling code CLOUDY 90.05 (Ferland et al. 1998) were used and a quasar ionizing spectrum assumed for the metagalactic radiation field. Some results are shown in Figure 5.

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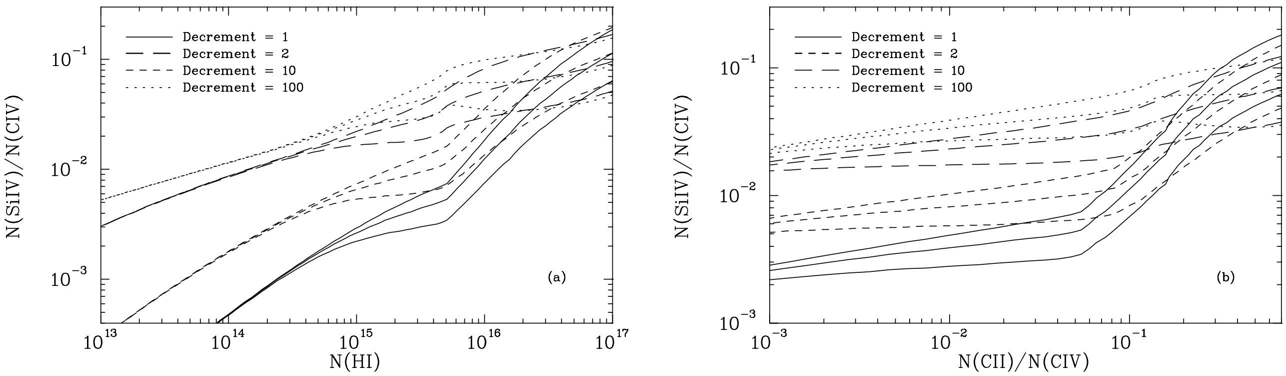

Fig. 5. Adapted from Savin (2000). *(a)* Predicted Si IV to C IV column densities versus H I column density. *(b)* Predicted ratio of Si IV to C IV column densities versus C II to C IV column densities. Each set of 3 curves represents a metagalactic radiation field with a decrement at 4 Ryd of 1 (solid curve), 2 (short-dashed curve), 10 (long-dashed curve), and 100 (dotted curve). For each set of three curves, the results are shown with the Si IV to Si III DR rate decreased by a factor of 2 (upper curve), unchanged (middle curve), and increased by a factor of 2 (lower curve).

Figure 5*a* shows that the Si/C abundance, inferred from ratios of Si IV to C IV column densities, could be up to ~ 2 times larger or smaller than that inferred using currently recommended DR rates. The Si/C ratio is used to constrain the initial mass function for the earliest generation of stars.

Figure 5*b* shows the predicted ratio of Si IV to C IV column densities versus C II to C IV column densities. This ratio is often used to constrain the magnitude of the decrement in the radiation field at 4 Ryd (the He II ionization edge). Accurately determining the magnitude of this decrement has a bearing on the issue of late He II reionization, which could significantly affect the temperature-density relation of the IGM and hence, the interpretation of Ly-α forest observations. The modeling demonstrates that the variation in the predicted Si IV/C IV ratio due to a factor of 2 uncertainty in the Si IV DR rate can be as large as that due to a factor of 10 change in the decrement.

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