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IONIZATION BALANCE, CHEMICAL ABUNDANCES, AND THE METAGALACTIC RADIATION FIELD AT HIGH REDSHIFT

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ABSTRACT

We have carried out a series of model calculations of the photoionized intergalactic medium (IGM) to determine the effects on the predicted ionic column densities due to uncertainties in the published dielectronic recombination (DR) rate coefficients. Based on our previous experimental work and a comparison of published theoretical DR rates, we estimate there is in general a factor of 2 uncertainty in existing DR rates used for modeling the IGM. We demonstrate that this uncertainty results in factors of ~1.9 uncertainty in the predicted N V and Si IV column densities, ~2.0 for O VI, and ~1.7 for C IV. We show that these systematic uncertainties translate into a systematic uncertainty of up to a factor of ~3.1 in the Si/C abundance ratio inferred from observations. The inferred IGM abundance ratio could thus be less than $(\mathrm{Si/C})_\odot$ or greater than $3(\mathrm{Si/C})_\odot$. If the latter is true, then it suggests the metagalactic radiation field is not due purely to quasars but includes a significant stellar component. Lastly, column density ratios of Si IV to C IV versus C II to C IV are often used to constrain the decrement in the metagalactic radiation field at the He II absorption edge. We show that the variation in the predicted Si IV to C IV ratio due to a factor of 2 uncertainty in the DR rates is almost as large as that due to a factor of 10 change in the decrement. Laboratory measurements of the relevant DR resonance strengths and energies are the only unambiguous method of removing the effects of these atomic physics uncertainties from models of the IGM.

Subject headings: atomic processes — cosmology: miscellaneous — diffuse radiation — intergalactic medium — quasars: absorption lines

1. INTRODUCTION

Many fundamental questions of cosmology can be addressed through observations of the Lyα forest. For example, observation of C IV, N V, O VI, and Si IV metal absorption lines can be used to constrain the spectral shape and history of the metagalactic radiation field, the chemical evolution of the universe, and the initial mass function (IMF) of the earliest generation of stars (Songaila & Cowie 1996; Giroux & Shull 1997; Boksenberg 1998; Songaila 1998). Interpreting spectra from the Lyα forest is carried out using both single-phase models (Giroux & Shull 1997; Songaila 1998) and cosmological models of the intergalactic medium (IGM) employing semianalytic approximations or hydrodynamical simulations (Miralda-Escudé et al. 1996; Bi & Davidsen 1997; Hellsten et al. 1997; Rauch, Haehnelt, & Steinmetz 1997; Zhang et al. 1997; Gnedin & Hui 1998; Riediger, Petitjean, & Mückert 1998; Madau, Haardt, & Rees 1999). These various models use different approximations and assumptions. However, one thing they all have in common is the need to calculate the ionization structure of the photoionized IGM. This is typically carried out using plasma codes that are written specifically for modeling the ionization structure of photoionized gas. One of the most commonly used codes for this purpose is CLOUDY (Ferland et al. 1998).

Fundamental to the accuracy of these plasma codes and any inferred astrophysical conclusions is calculating the correct ionization balance. This requires reliable photoionization (PI), radiative recombination (RR), and dielectronic recombination (DR) rate coefficients. Recent Opacity Project (OP) calculations for near-threshold PI of valence-shell electrons, in combination with Hartree-Dirac-Slater calculations for energies far above threshold and for inner-shell electrons, have provided what are believed to be highly accurate PI cross sections (Seaton et al. 1992; Verner et al. 1996; Ferland et al. 1998). The effects of the new OP cross sections on IGM models have been investigated by Donahue & Shull (1991). As for the relevant recombination rates, at IGM temperatures (~10^4 K) the DR rate is nearly an order of magnitude larger than the RR rate for most ions, including C IV, N V, O VI, and Si IV (Arnaud & Rothenflug 1985; Arnaud & Raymond 1992; Kallman et al. 1996). Uncertainties in the relevant RR rates are thus expected to have an insignificant effect on the predicted ionization structure of the IGM for these ions.

In this paper we demonstrate that uncertainties in the DR rates for C IV, N V, O VI, and Si IV significantly hamper our ability to constrain reliably the chemical abundances and the shape of the metagalactic radiation field at high redshift. In § 2 we review the status of the relevant DR rates and their uncertainties. The model we use to calculate the ionization structure of the IGM is presented in § 3. In § 4 we present the results of our simulations, demonstrate the effects of the estimated uncertainties in the DR rates, and discuss the astrophysical implications. We present our conclusions in § 5.

2. DIELECTRONIC RECOMBINATION

The lack of reliable DR rates is the dominant uncertainty in ionization balance calculations of photoionized plasmas (Ferland et al. 1998). A critical evaluation of published theoretical DR rates suggests that a factor of 2 or more uncertainty is inherent in the different theoretical techniques used to calculate DR for ions with partially filled L or M shells (Arnaud & Raymond 1992; Savin et al. 1997, 1999). This is supported by laboratory measurements that have turned up errors of factors of 2 to orders of magnitude in calculated DR rates (Linkemann et al. 1995; Savin et al. 1997, 1999;

Schippers et al. 1998). The measurements also demonstrate that it is not possible a priori to know which set of calculations, if any, will agree with experiment. Taken all together, these results suggest that, for ions with partially filled L or M shells, a factor of ~2 uncertainty exists in almost all published theoretical DR rates currently used for modeling photoionized plasmas.

The recent claim of Nahar & Pradhan (1997) that the overall uncertainty in their electron-ion recombination data is ~10%–20% has sown a certain amount of confusion as to the true state of theoretical DR rates. Their statement applies primarily to DR rates for K shell ions and relates only to calculations that have been carried out taking fine structure into account (i.e., non–*LS*-coupling calculations). The statement does not apply to the majority of their work, which has been carried out in *LS* coupling.

LS-coupling calculations are known not to include all possible autoionization levels contributing to the DR process. As a result such calculations provide only a lower limit for the DR rate (Badnell 1988). For example, for DR at $T_e = 10^4$ K onto boron-like C II, N III, and O IV, intermediate coupling (IC) calculations, which include *LS*-forbidden autoionizing levels, yielded rates ~70% larger than the *LS*-coupling rates (Badnell 1988). For lithium-like ions, Griffin, Pindzola, & Bottcher (1985) showed that *LS* coupling accounts for only two-thirds of all possible recombining channels. IC calculations yield a DR rate for lithium-like C IV that is 50% larger than the *LS*-coupling rate. Recent storage-ring measurements and relativistic many-body perturbation calculations have verified the breakdown of *LS* coupling for C IV (Mannervik et al. 1998).

As an example of the state of DR theory, we show in Figure 1 the published theoretical rates for $\Delta n = 0$ DR onto C IV. A comparison of these rates gives a good overview of the state of DR theory. The oldest rate is from the semi-empirical Burgess (1965) formula. It was designed to provide high-temperature DR rates and not surprisingly does not reproduce the low-temperature behavior. Here the Burgess rate peaks at a value larger than all the other theoretical rates. For Fe XIX, the Burgess rate peaked at a value lower than all other theoretical rates (Savin et al. 1999). This suggests that it is not possible to know a priori whether the Burgess rate will lie at the lower or upper limit of theoretical DR rates (or somewhere in between).

The rate from Shull & Van Steenberg (1982) is derived from the *LS*-coupling calculations of Jacobs, Davis, & Rogerson (1978) and does not account for those DR channels important at low temperatures. The Nussbaumer & Storey (1983) *LS*-coupling calculations were carried out to provide reliable low-temperature DR rates. Also shown in Figure 1 are the *LS*-coupling calculations of McLaughlin & Hahn (1983) and Romanik (1988). These calculations were all carried out using single-configuration models. There is nearly a factor of 2 scatter between the various calculations.

Modern techniques for calculating DR rates include the multiconfiguration Breit-Pauli method using IC (Badnell 1989), the fully relativistic, multiconfiguration Dirac-Fock method (Chen 1991), and the unified RR + DR ***R***-matrix method (Nahar & Pradhan 1997). It is clear from Figure 1 that the calculations of Badnell (1989) and Chen (1991) were carried out only for high-temperature plasmas. The rates of Nahar & Pradhan (1997) were carried out for all temperatures but were, unfortunately, carried out using *LS* coupling and thus should be multiplied by a factor of 1.5. This brings their rates into rough agreement with the DR rates of Romanik at ~10^4 K and with the Burgess formula at higher temperatures. Thus even the modern techniques for calculating DR rates show nearly a factor of 2 spread.

Also plotted in Figure 1 is the RR rate of Péquignot, Petitjean, & Boisson (1991). At 400 K ($k_B T_e \sim 0.034$ eV), the

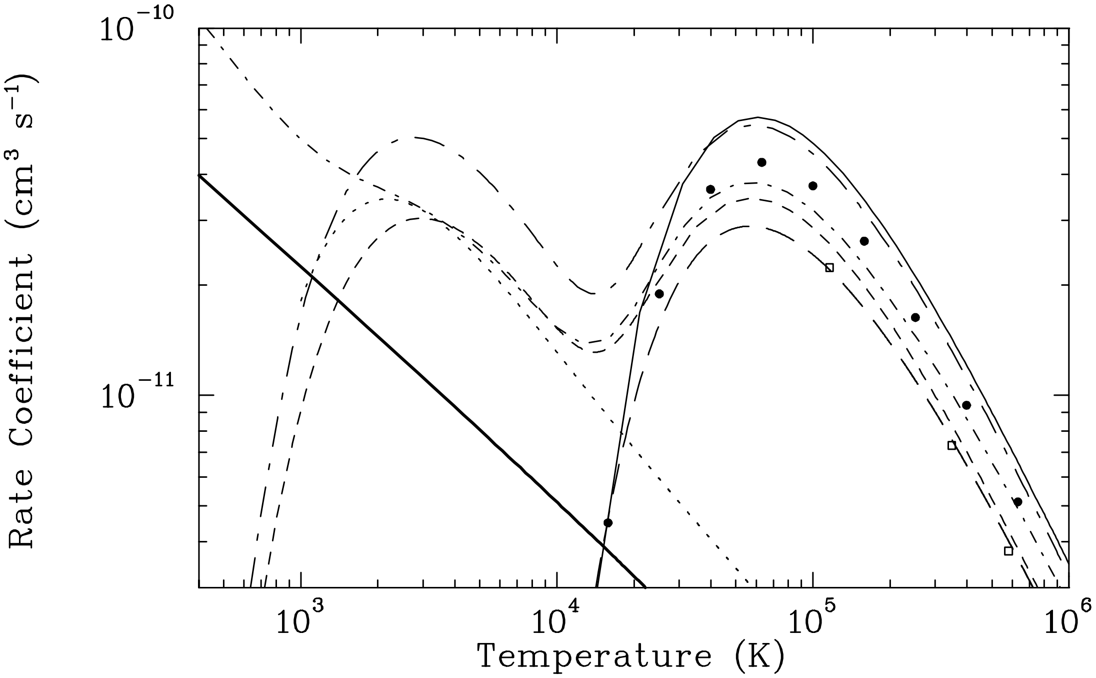

FIG. 1.—Published theoretical C IV to C III $\Delta n = 0$ DR rates vs. electron temperature. Calculations are from Burgess (1965) (*thin solid curve*); Shull & Van Steenberg (1982) (*long-dashed curve*); Nussbaumer & Storey (1983) (*short-dashed curve*); McLaughlin & Hahn (1983) (*medium-dashed curve*); Romanik (1988) (*dot–long-dashed curve*); Badnell (1989) (*circles*); Chen (1991) (*squares*); and Nahar & Pradhan (1997), who calculated a combined radiative recombination (RR) and DR rate (*dot–medium-dashed curve*). The thick solid curve is the RR rate from Péquignot et al. (1991).

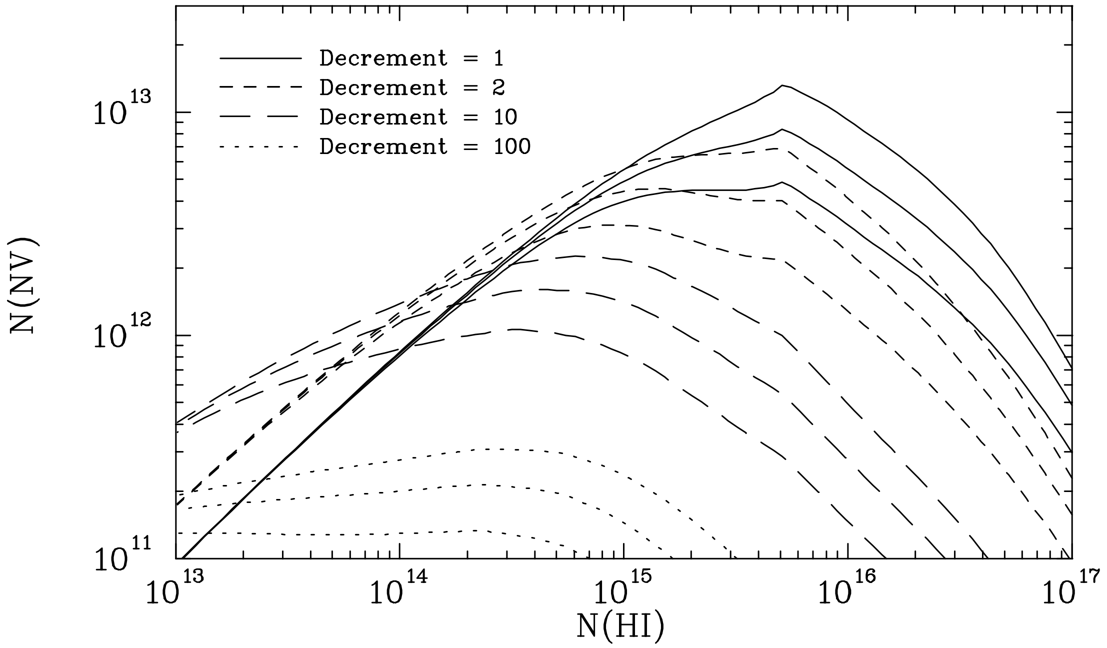

FIG. 2.—Predicted N V column density vs. H I column density for the model described in § 3. Each set of three curves represents a metagalactic radiation field with a decrement at 4 ryd of 1 (*solid curves*), 2 (*short-dashed curves*), 10 (*long-dashed curves*), and 100 (*dotted curves*). We have also varied the N V to N IV DR rate and left the other rates unchanged. For each set of three curves, the results are shown with the rate decreased by a factor of 2 (*upper curve*), unchanged (*middle curve*), and increased by a factor of 2 (*lower curve*).

RR + DR rate of Nahar & Pradhan (1997) is over a factor of 2 larger than that of Péquignot, Petitjean, & Boisson. This is not likely to be due to interference effects between RR and DR. The lowest lying *LS*-allowed DR resonance in C IV has been measured to fall at ~0.29 eV (Mannervik et al. 1998). This is 8.5 *e*-folding factors above 400 K. The recombination rate of Pradhan & Nahar at 400 K should thus be due entirely to nonresonant RR. The source of this discrepancy remains unclear.

Consisting of one electron outside of a closed shell, C IV is one of the simplest ions to treat theoretically and there have been numerous DR calculations, but theory clearly has yet to converge. For many ions there are no published DR rates calculated using state-of-the-art techniques. Only single-

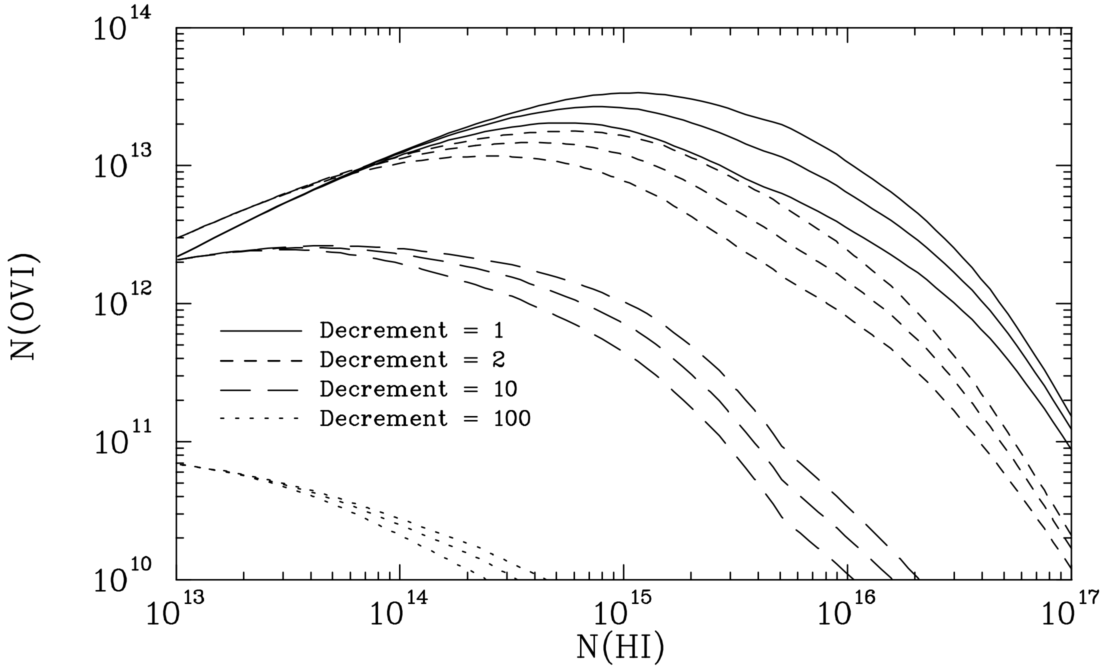

FIG. 3.—Predicted O VI column density vs. H I column density. We have varied the O VI to O V DR rate and left the other rates unchanged. See Fig. 2 for further details.

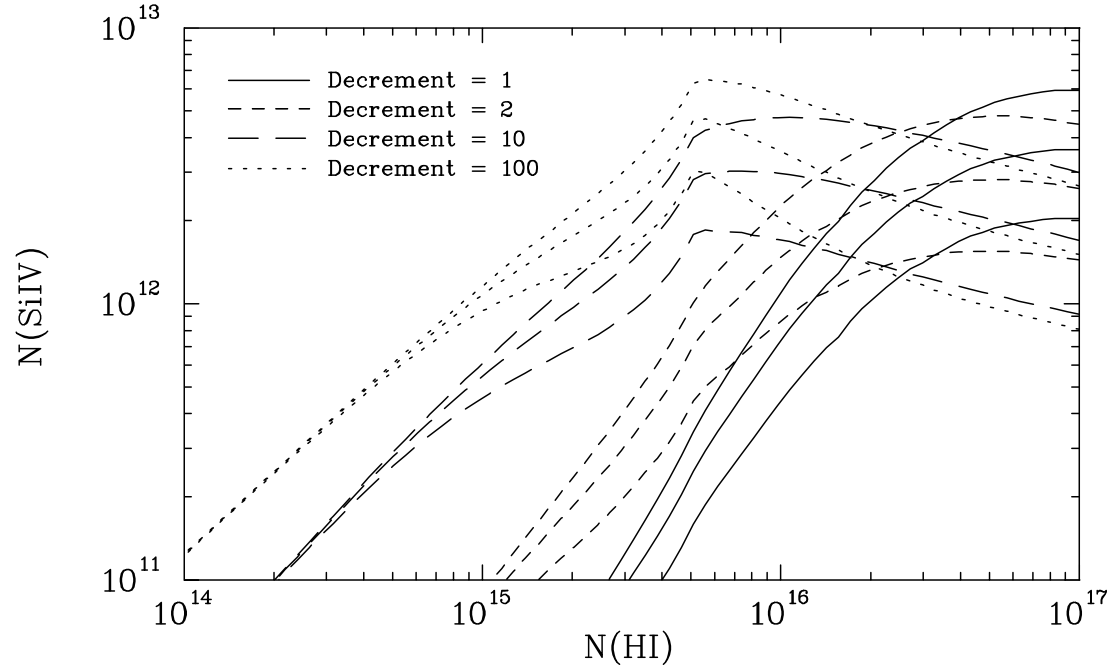

FIG. 4.—Predicted Si IV column density vs. H I column density. We have varied the Si IV to Si III DR rate and left the other rates unchanged. See Fig. 2 for further details.

configuration *LS*-coupling calculations or Burgess rates exist. The above comparison shows that even if modern calculations did exist, they would still probably not have converged.

Laboratory measurements are needed in order to determine the true DR rates and the best theoretical techniques for calculating DR. But, as demonstrated by Savin et al. (1999), it is not possible to distinguish between different theoretical techniques based solely on the comparison of rate coefficients with experiments. The only unambiguous way to benchmark DR theory is through a detailed comparison of resonance strengths and energies.

N V, O VI, and Si IV are similar to C IV in that they consist of one electron outside of a closed shell. Based on our experimental studies and theoretical comparisons, we estimate a factor of 2 uncertainty in the calculated rates for DR onto N V, O VI, and Si IV. DR onto C IV has recently been measured by Mannervik et al. (1998) and Schippers (1999)

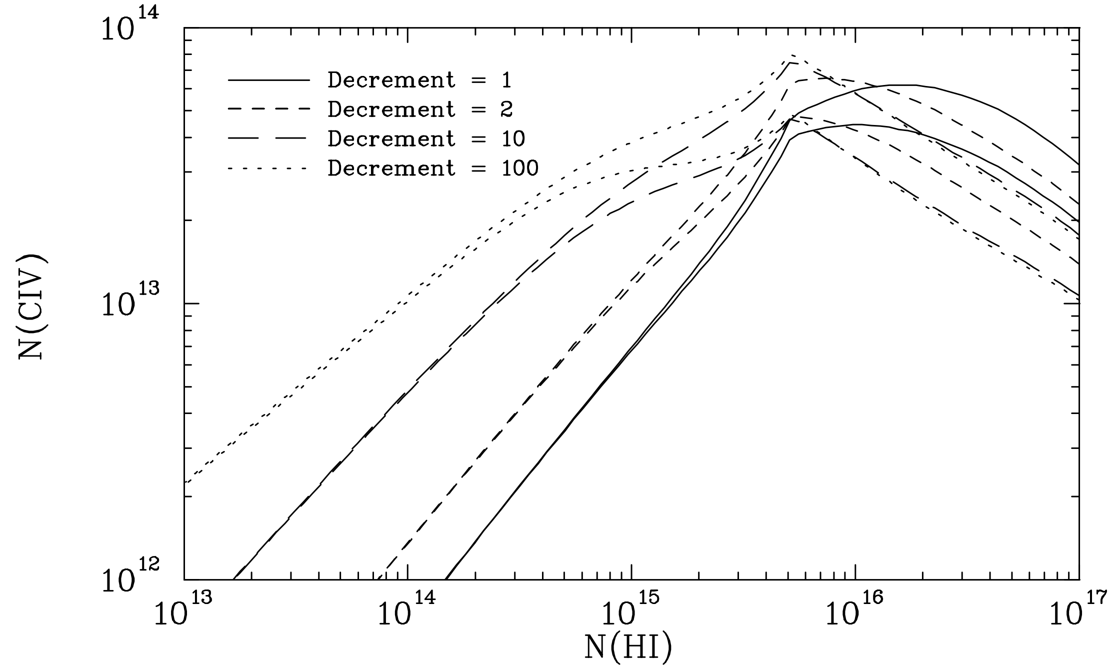

FIG. 5.—Predicted C IV column density vs. H I column density. We have varied the C IV to C III DR rate and left the other rates unchanged. For each set of curves, the results are shown for the rate unchanged (*upper curve*) and increased by a factor of 2 (*lower curve*). See Fig. 2 for further details.

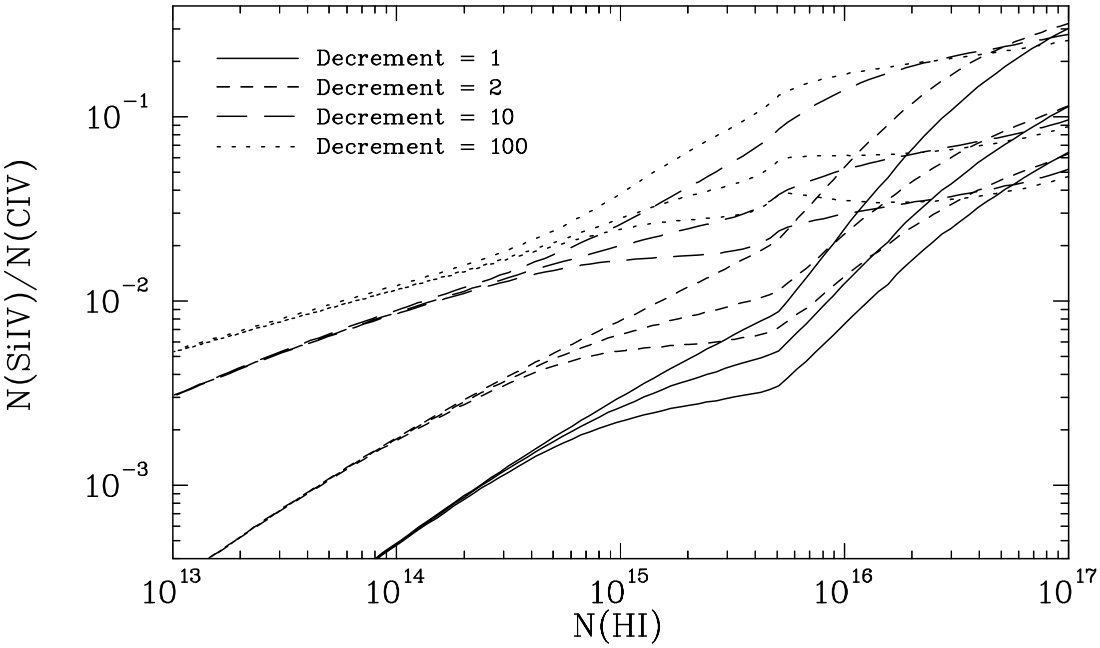

FIG. 6.—Predicted Si IV to C IV column densities vs. H I column density. We have varied the C IV and Si IV DR rates and left the other rates unchanged. For each set of three curves, we have decreased the Si IV rate by a factor of 2 and increased the C IV rate by a factor of 2 (*upper curve*), left both rates unchanged (*middle curve*), and increased the Si IV rate by a factor of 2 while leaving the C IV rate unchanged (*lower curve*). See Fig. 2 for further details.

and his collaborators. These groups are working to generate new C IV DR rates.

3. MODEL

Hellsten et al. (1998) have carried out hydrodynamic cosmological simulations for a redshift of $z = 3$. They present the resulting relationships for electron temperature T_e versus total hydrogen density $n_{\rm H}$ and for $n_{\rm H}$ versus H I column density $N_{\rm H\,I}$. We use their results, along with CLOUDY version 90.05, to investigate the effects of the uncertainty in the C IV, N V, O VI, and Si IV DR rates on the predicted IGM column densities for these ions. The temperature-density relation depends partly on the ionization structure of the gas and hence on the DR rates used. To simulate the possible effects the DR uncertainties have on this relation, we have also carried out calculations with T_e increased and decreased by a factor of 2. This does not significantly affect the conclusions in this paper.

We use the same spectral shape for the metagalactic radiation field as Hellsten et al. (1998) but have varied the decre-

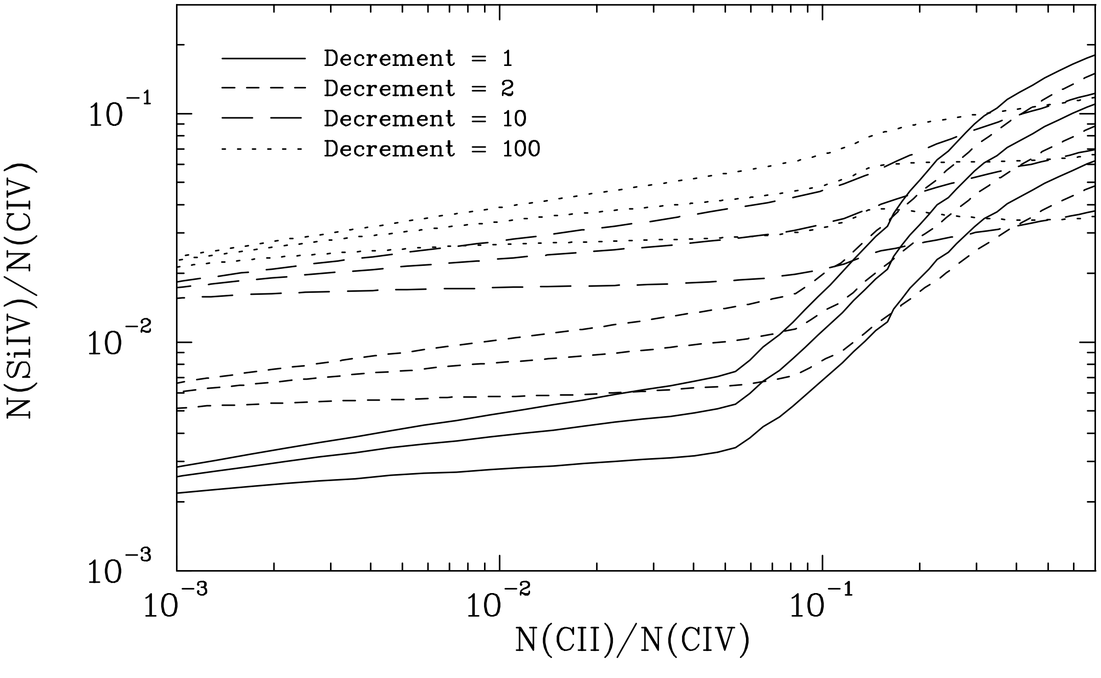

FIG. 7.—Ratio of Si IV to C IV column densities vs. C II to C IV column densities. We have varied the Si IV to Si III DR rate and left the other rates unchanged. See Fig. 2 for further details.

ment at the He II absorption edge (4 ryd) by factors of 1, 2, 10, and 100. We assume that the decrement at the 4 ryd edge does not affect the temperature-density relationship. This assumption is not strictly valid. Hui & Gnedin (1997) have shown that a decrement of 10^4 (twice our maximum decrement) does decrease the temperature but by less than a factor of 2. Our modeling shows that this uncertainty in the temperature-density relationship does not significantly affect the conclusions in this paper.

We use a flux at 912 Å of $J_\nu = 10^{-21}$ ergs cm^{-2} s^{-1} sr^{-1} Hz^{-1}. For a metallicity, we use $[Z/H] \equiv \log(n_Z/n_H) - \log(n_Z/n_H)_\odot = -2$. At $N_H \gtrsim 10^{17}$ cm^{-2}, the IGM begins to become optically thick and the self-shielding of the UV radiation needs to be taken into account (Rauch et al. 1997). Here we restrict our calculations to $N_H \leq 10^{17}$ cm^{-2}.

4. SIMULATIONS AND ASTROPHYSICAL IMPLICATIONS

To simulate the effects of the uncertainties in the DR rates, we have run CLOUDY with the rates onto N V, O VI, and Si IV decreased by a factor of 2, unchanged, and increased by a factor of 2. For a plasma in LTE, detailed balance would require a corresponding change in the resonant portion of the PI rates out of excited states. However, here we are concerned with ground-state ions under non-LTE conditions. Hence, changes to the relevant PI rates out of excited states are unimportant.

Figures 2, 3, and 4 show the resulting $N_{\rm N\,V}$, $N_{\rm O\,VI}$, and $N_{\rm Si\,IV}$ versus $N_{\rm H\,I}$. The resulting column densities differ from the column densities predicted using the unchanged DR rates by factors of up to ∼1.9 for N V and Si IV and 2.0 for O VI. This translates into a factor of up to ∼2.0 uncertainty in any derived abundance.

For C IV, CLOUDY uses the low-temperature DR rates of Nussbaumer & Storey (1983) and the high-temperature DR rates of Shull & Van Steenberg (1982). These rates lie at the lower end of the range of published C IV DR rates. We use the C IV DR rates unchanged and also increased by a factor of 2. Figure 5 shows the resulting $N_{\rm C\,IV}$ versus $N_{\rm H\,I}$. The predicted column density can be as much as a factor of ∼1.7 smaller than that predicted using the unchanged DR rates. This could increase any inferred abundances by up to a factor of 1.7.

In Figure 6 we have plotted the predicted $N_{\rm Si\,IV}/N_{\rm C\,IV}$ ratio versus $N_{\rm H\,I}$. Here we vary the Si IV and C IV DR rates. The resulting ratio could be up to 1.9 times smaller or 3.1 times larger than the ratio predicted using the unchanged DR rates. Hence, the inferred Si/C abundance ratio could be up to 3.1 times smaller or 1.9 times larger than that inferred using the unchanged DR rates.

The inferred Si/C ratio for the IGM is used to constrain the IMF of the earliest generation of stars. Giroux & Shull (1997) inferred a relative abundance ratio for the IGM of Si/C ∼ 2(Si/C)$_\odot$. Results such as those shown in Figure 6 indicate that uncertainties in the DR rates can make Si/C either less than (Si/ C)$_\odot$ or greater that 3(Si/C)$_\odot$. However, Woosley & Weaver (1995) have shown that, even if massive stars dominate the IMF, chemical evolution models with Si/C > 3(Si/C)$_\odot$ are unrealistic. Abundance ratios this large would, thus, suggest that the metagalactic radiation field is not purely due to quasars but includes a significant component from stellar radiation (Giroux & Shull 1997).

In Figure 7 we have plotted the predicted $N_{\rm Si\,IV}/N_{\rm C\,IV}$ versus $N_{\rm C\,II}/N_{\rm C\,IV}$. Comparisons between the observed ratios and model predictions are often used to constrain the magnitude of the decrement in the radiation field at 4 ryd. The magnitude of the decrement affects the amount of He II photoionization heating of the IGM. Accurately determining this decrement has a direct 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 Lyα forest observations (Miralda-Escudé & Rees 1992; Hui & Gnedin 1997). Many of the measured ratios fall in the range of $10^{-2} \lesssim N({\rm C\,II})/N({\rm C\,IV}) \lesssim 10^0$ (Songaila & Cowie 1996; Boksenberg 1998; Songaila 1998). Our models demonstrate that in this range the variation in the predicted $N_{\rm Si\,IV}/N_{\rm C\,IV}$ ratio due to a factor of 2 uncertainty in the DR rates can be as large as that due to a factor of 10 change in the decrement.

5. CONCLUSIONS

We have shown the effects on IGM models due to the estimated uncertainties in the DR rates. These uncertainties limit our ability to constrain the chemical abundances and the shape of the metagalactic radiation field at high redshift. Measurements of the relevant DR resonance strengths and energies are the only unambiguous way to remove these atomic physics uncertainties.

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