CHEMISTRY IN THE EARLY UNIVERSE

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ABSTRACT. Galaxies and the first stars in the universe formed billions of years ago as a result of the cooperative effects of gravitational collapse and nonequilibrium chemistry. Gravity drew the primordial gas together into lumps; the formation of the first molecules in the universe, simple diatomic molecules like H_2, H_2^+, HD, HeH^+, LiH, and LiH^+, may then have ensured that the heat generated by gravitational collapse and shock waves was radiated away rapidly enough to allow the gravitational collapse and fragmentation of these gaseous lumps to proceed to the point of forming stars and galaxies. We briefly mention a few of the latest studies of this primordial chemistry, including that in the evolving intergalactic medium (IGM) in a Cold Dark Matter (CDM) model cosmology and that in radiative shocks in the early universe.

1. Introduction

Molecule formation in the early universe has been studied under three related circumstances: (1) the uniform pregalactic IGM at high redshift z in the postrecombination epoch ($z \lesssim 10^3$)[1-4]; (2) the gravitational collapse of primordial gas clouds [5-16]; and (3) the radiative shocks which occur in a wide range of galaxy and primordial star formation theories [17-29]. In view of the space limitation here, I will just mention a few highlights of work completed since the last reviews of this subject [25,30] and refer the reader to those reviews for the full background and references.

When the universe recombined at $z \sim 10^3$, the gas was composed primarily of H, D, ^{4}He, ^{3}He, and ^{7}Li, with nuclear abundances by number relative to H of order 1, 5×10^{-5}, 10^{-1}, 10^{-5}, and 10^{-10}, respectively [31]. In this essentially metal-free

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gas, H_2 was likely to have been the most abundant molecule and was potentially important as a source of radiative cooling in collapsing pregalactic clouds and in shock-heated pregalactic gas. Since H_2 has no dipole moment, formation by direct radiative association of two H atoms is very slow, and H_2 formation is thought to have been dominated, instead, by the creation of H^- by radiative attachment, followed by associative detachment [5,6]:

$$H + e^- \rightarrow H^- + \gamma$$

$$H + H^- \rightarrow H_2 + e^-$$
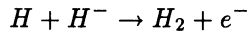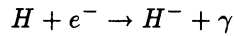
and by the creation of H_2^+ by radiative association, followed by charge transfer [32]:

$$H + H^+ \rightarrow H_2^+ + \gamma$$

$$H_2^+ + H \rightarrow H_2 + H^+.$$
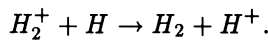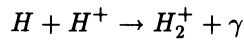
2. H_2 in the IGM in a Postrecombination CDM Universe

Previous studies of molecule formation in the pregalactic IGM beginning with the recombination epoch at $z \cong 10^3$ considered a uniform expanding IGM of fixed comoving density Ω_{IGM} (in units of the critical density for an Einstein-deSitter universe) and focused on the epoch prior to nonlinear structure formation in the universe [1,2]. (An exception is [3], which considered the effect of radiation from postulated primordial stars at high z.) As part of our general study of the IGM, we have reconsidered this problem within the context of the recently popular CDM model for galaxy and large-scale structure formation. We have coupled our detailed, numerical calculations of the thermal and ionization balance, molecule formation, and radiative transfer in a uniform IGM of H and He to the linearized equations for the growth of density fluctuations in both the gaseous and dark matter components [4,33,34]. The mean IGM density parameter in this case is $\Omega_{IGM}(z) = \Omega_b[1-f_c(z)]$, where Ω_b is the total baryon mass fraction in the universe and $f_c(z)$ is the time-varying, collapsed baryon fraction. We consider a standard CDM model with $\Omega_{tot} = 1$, $\Omega_b = 0.1$, and Hubble constant $h = H_o/(100\ km\ s^{-1}\ Mpc^{-1}) = 0.5$, with a power spectrum normalized so that the rms density fluctuation evaluated using a "top-hat" filter is $\sigma_o = 1/b$ at $R = 8h^{-1}$ Mpc at present, where b is the so-called bias parameter. In order to account for the observed absence of a detectable H Ly α absorption trough in the spectra of high z quasars due to a smoothly distributed IGM (so-called Gunn-Peterson effect; "GP"), we assume that the collapsed fraction

releases just enough ionizing radiation at a constant rate per collapsed baryon, with an AGN-like spectrum ($F_\nu \propto \nu^{-1.5}$), to reduce the GP optical depth to less than 0.1 by $z = 4.1$. This minimal emissivity corresponds to 1200 ($b = 1$) or 24,400 ($b = 2.6$) ionizing photons per collapsed baryon per present Hubble time.

Shown in Figure 1 are some results of our calculations, which solve rate equations for the concentrations of H^o, H^+, He^o, He^+, He^{++}, H_2, H_2^* (vibrationally excited), H_2^+, H^-, and e^-, the energy conservation equation, including the effects of cosmological expansion, radiative cooling, and cooling (or heating) by Compton scattering of the cosmic microwave background (CMB), and the equation of radiative transfer, including the opacity of the IGM and its own diffuse emission, as well as the mean opacity of an evolving distribution of gas clumps (i.e. quasar absorption-line clouds) embedded in the smoothly distributed IGM. As in previous studies, H_2 formation shortly after recombination was limited by the photodestruction of H^- and H_2^+ by the CMB. It is important in this case to take account of the population of excited states of H_2^+ with an excitation temperature equal to the CMB radiation temperature. Otherwise, photodissociation of H_2^+ at high z is underestimated, and H_2 formation is spuriously accelerated and enhanced. For 200 $\lesssim z \lesssim 600$, the H_2^+ process dominated the formation of H_2, yielding a concentration $\lesssim 10^{-6}$ by $z \sim 300$. By $z \sim 100$, the H^- process boosted this to $\sim 2 \times 10^{-6}$, before the collapsed fraction finally released enough radiation by $z \lesssim 25$ ($b = 2.6$) or $z \lesssim 50$ ($b = 1$) to heat and ionize the IGM, destroying the H_2. Figure 1 shows that once IGM reionization began, unshielded photodissociation would have destroyed the H_2 more quickly than collisional dissociation, but even in the fully self-shielded limit (no photodissociation), collisions would have been more than enough to reduce the H_2 concentration by many orders of magnitude to undetectable levels even before the GP constraint was satisfied.

3. Radiative Shocks and Nonequilibrium H_2 Chemistry in the Early Universe

Shock waves in a metal-free gas are predicted to occur in the IGM and inside protogalaxies under a wide range of circumstances in the theory of galaxy and primordial star formation, including gravitational collapse of density fluctuations, cloud-cloud collisions, and blast waves from the explosive heating of the IGM. In all cases, the radiative cooling of the postshock gas is essential in order to dissipate enough gravitational or explosion energy to make gravitational instability and fragmentation possible in the shock-heated gas, a prerequisite for galaxy or star
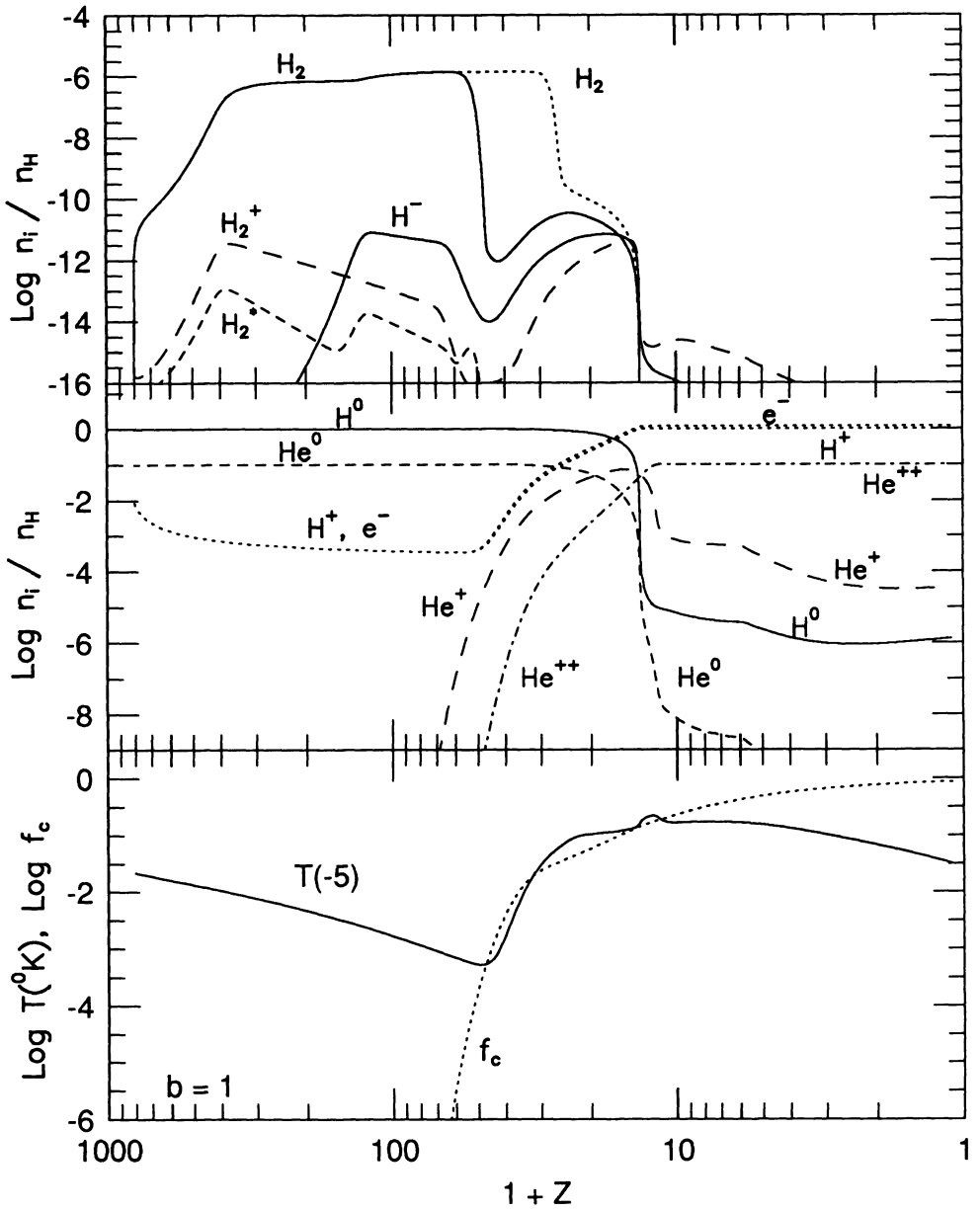
Figure 1. IGM temperature $T(^\circ K)(\times 10^{-5})$, collapsed baryon fraction f_c, and species concentration by number relative to H, n_i/n_H, as labeled for bias $b = 1$. Solid curve for H_2 assumes unshielded photodissociation; dashed H_2 curve neglects photodissociation.

formation. We have numerically solved the hydrodynamical conservation equations, along with the rate equations for nonequilibrium ionization, recombination, molecule formation and dissociation, and the equation of radiative transfer, in detail for steady-state, planar shocks of velocity in the range $20 \leq v_s \leq 400$ km s^{-1} for a range of conditions appropriate for shocks in the IGM and inside protogalaxies [22-29]. (Calculations for shocks in the IGM were also reported by [20].) We include the same species as in the calculations for Figure 1. Figure 2 shows results for shocks inside protogalaxies, with $v_s = 300$ km s^{-1} such as would be produced by the typical gravitationally-induced motions within a protogalaxy, in a gas of preshock density $n_{H,1} = 0.1$. The shocked gas generally cools faster than it can recombine and, as a result, is able to form an H_2 concentration as high as 10^{-3} or higher via the H^- and H_2^+ processes, thanks to the enhanced nonequilibrium ionization at 10^4K. With such an H_2 concentration, the gas cools rapidly by H_2 rotational-vibrational line excitation to $T \sim 10^2 - 10^3$K, well below the canonical final temperature of 10^4K for a molecule-free gas without metals. This cooling below 10^4K significantly lowers the characteristic gravitationally unstable fragment mass for such shocks, relative to the value if the gas cooling stops at 10^4K.

This presents a problem for the suggestion that globular clusters formed within protogalaxies by gravitational instability in the compressed gas resulting from radiative shocks with velocities of the order of the virial velocity of the protogalaxy or from thermal instability in gas at the virial temperature [35,36]. Under such circumstances, gas which cools to 10^4K and, thereafter, remains at 10^4K for a time longer than its internal free-fall time will lead naturally to gravitational instability with a characteristic mass comparable to those of globular clusters. If, instead, the gas forms enough H_2 to cool too rapidly below 10^4K, however, the model fails. Our shock calculations have led to a new version of the model, in which a strong enough UV or soft X-ray source ($L \gtrsim 10^{45}$ erg s^{-1}), such as a quasar or early-type stars, is required to be present within the protogalaxy during the globular cluster formation epoch to suppress H_2 formation in the shocks [26].

Figure 3 shows the effect of adding to the shock in Figure 2 a preshock magnetic field of strength $B_1 = 1$ μG, oriented parallel to the shock front [29]. Flux-freezing and the nearly isobaric compression of the radiatively cooling postshock gas together cause magnetic pressure to dominate downstream before the gas reaches $\sim 10^4$K. This halts the compression and makes the photon-to-atom ratio higher in the temperature plateau at 10^4K than in the nonmagnetic case. The latter encourages the photodestruction of H_2 and makes it easier to suppress H_2 formation and cooling with a given radiation flux level than in the nonmagnetic case, thereby lowering the threshold level required for the globular cluster formation model (e.g. $L \sim 10^{44}$ erg s^{-1} or less, for $B_1 \gtrsim 1.6$ $n_{H,1}^{1/2}$ μG).
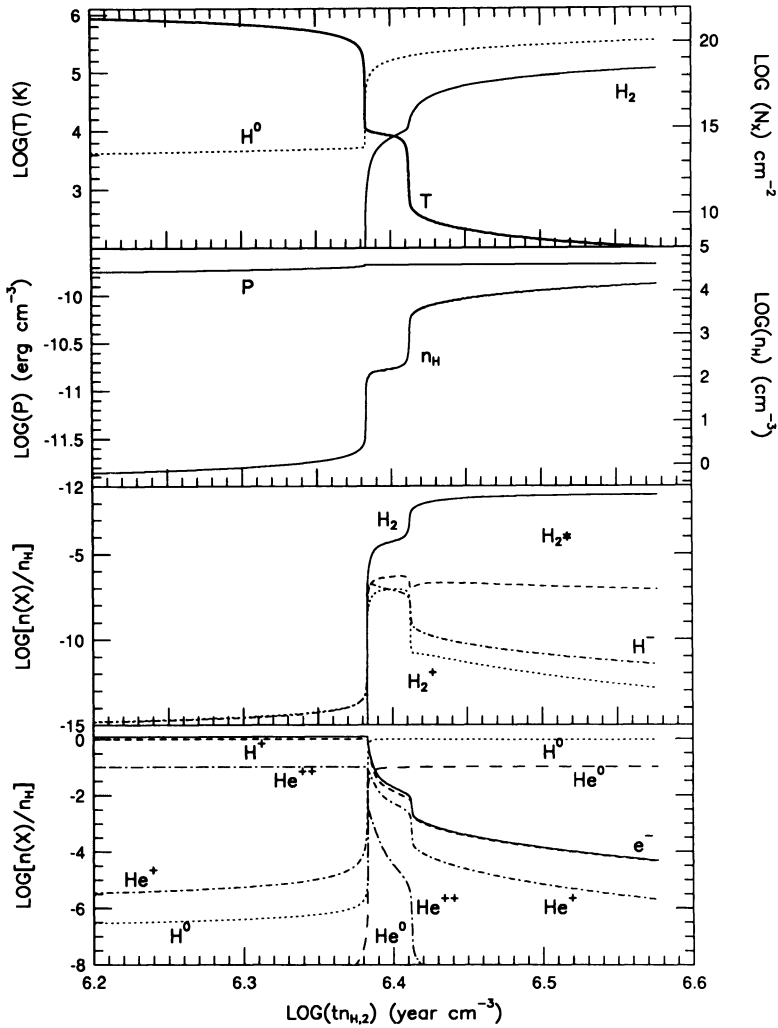
Figure 2. Postshock flow quantities versus $tn_{H,2}$ (years cm^{-3}) for $v_s = 300$ km s^{-1} and $n_{H,1} = 0.1$ cm^{-3}, where $n_{H,2}$ is postshock H atom density and t is time since fluid element was shocked. Horizontal coordinate also corresponds to N_H cm^{-2}, total H column density between fluid element and shock, at time t, where $N_H = n_{H,1}v_s t = (n_{H,1}/n_{H,2})$ $v_s tn_{H,2}$, as long as we take $log_{10}N_H = log_{10}(tn_{H,2}) + 14.382$. Top panel shows temperature (scale at left) and total H^0 and H$_2$ column densities between fluid element and shock (scale at right) as labeled. Second panel shows gas pressure (scale at left) and H atom density (scale at right) as labeled. Third and fourth panels show concentrations n_i/n_H as labeled.
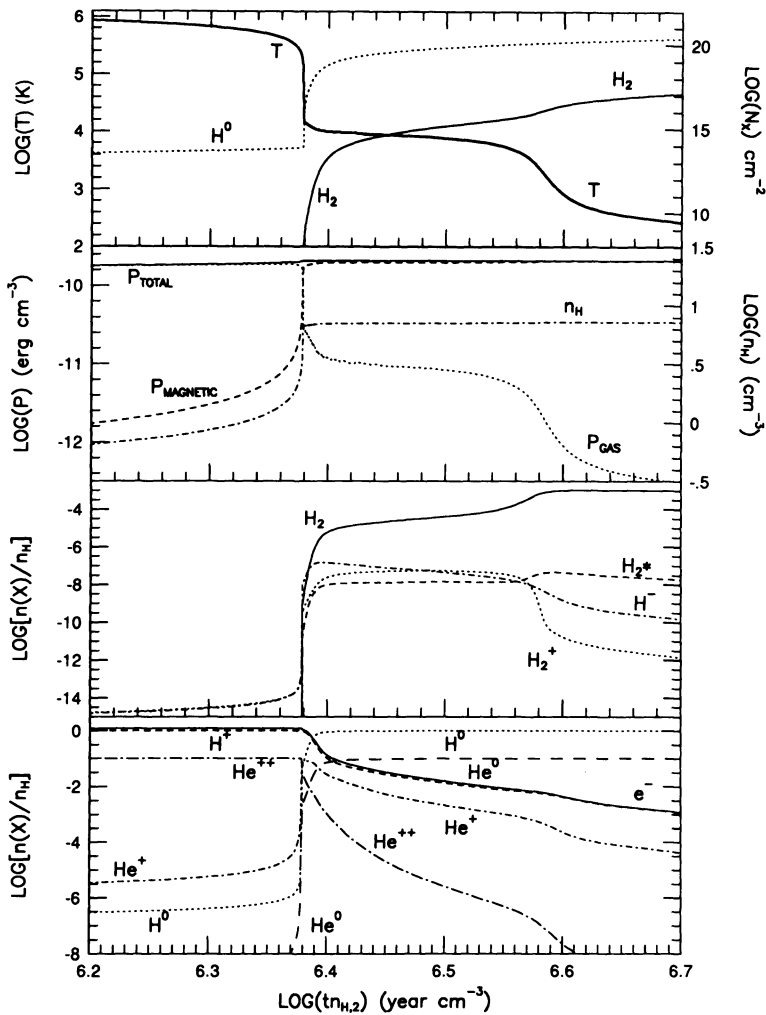
Figure 3. Same as Figure 2, but magnetized case with $B_1 = 1\mu G$. All panels are the same as in Figure 2 except the second, where gas, magnetic and total pressure are plotted, along with H atom density.

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QUESTIONS AND ANSWERS

L.Blitz: I thought that the lowest temperature you could cool pure H_2 gas was $\sim$500 K which is the temperature of the lowest quadrupole H_2 rotational transition. Your curves level off at temperatures a little more than 100 K. Where does the other factor of 4 - 5 in the temperature come from?

P.R.Shapiro: Although it is true that the lowest quadrupole rotational transition for H_2 corresponds to an excitation energy of 510 K (in temperature units), this only means that the collisional excitation rate for this transition is exponentially cut-off at temperatures below 510 K. Hence, while the rate is reduced by this exponential T dependence, it is not zero. Another words, the high energy tail of the H atom Maxwellian velocity distribution still has enough energy per atom to excite the H_2 transition. In addition, in our post shock gas, as the temperature drops below 500 K, the H_2 concentration continues to increase, so this offsets the exponential fall-off of the T dependence of the excitation cooling rate per H_2 molecule.