

H_3^+ cooling in primordial gas

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Simulations of the thermal and dynamical evolution of primordial gas typically focus on the role played by H_2 cooling. H_2 is the dominant coolant in low-density primordial gas and it is usually assumed that it remains dominant at high densities. However, H_2 is not an effective coolant at high densities, owing to the low critical density at which it reaches local thermodynamic equilibrium and to the large opacities that develop in its emission lines. It is therefore important to quantify the contribution made to the cooling rate by emission from the other molecules and ions present in the gas. A particularly interesting candidate is the H_3^+ ion, which is known to be an effective coolant at high densities in planetary atmospheres. In this paper, we present results from simulations of the thermal and chemical evolution of gravitationally collapsing primordial gas, which include a detailed treatment of H_3^+ chemistry and an approximate treatment of H_3^+ cooling. We show that in most cases, the contribution from H_3^+ is too small to be important, but if a sufficiently strong ionizing background is present, then H_3^+ cooling may become significant.

Keywords: astrochemistry; molecular processes; cosmology; theory

1. Introduction

Developing an understanding of the chemical and thermal behaviour of dense primordial gas is a key step in understanding how the first stars in the Universe formed. Detailed modelling of the evolution of the first star-forming protogalaxies using high-resolution, adaptive mesh simulations (Abel *et al.* 2000, 2002) has taught us much about their properties, but for reasons of computational efficiency, these models have generally included only a small fraction of the full range of chemistry possible in primordial gas. This approach is generally justified by the argument that since H_2 is the dominant coolant at low densities and its formation in high-density gas is very efficient, owing to three-body formation processes such as



then H_2 should also be the dominant coolant at high densities. However, it is not immediately obvious that this is actually the case. At densities above $n_{\text{cr}} \sim 10^4 \text{ cm}^{-3}$, the cooling rate per H_2 molecule quickly becomes independent of the gas density as the H_2 level populations approach their local thermodynamic equilibrium (LTE) values. For number densities $n \gg n_{\text{cr}}$, the effectiveness of H_2 as a coolant is therefore

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strongly suppressed relative to coolants which reach LTE at much higher densities. Moreover, cooling from H_2 is further suppressed at densities $n > 10^9 \text{ cm}^{-3}$ by the development of large optical depths in its emission lines (Ripamonti & Abel 2004). It is therefore important to determine whether cooling from any other molecular species present in the gas can become competitive with H_2 cooling at high densities.

The molecular ion H_3^+ is a particularly interesting candidate. It is known to be an important coolant in other high-density environments, such as the atmosphere of Jupiter (Miller *et al.* 2000), and calculations of its LTE cooling function (Neale *et al.* 1996) show that in the LTE limit it provides several orders of magnitude more cooling per molecule than H_2 . Moreover, H_3^+ does not react with H_2 and is not easily destroyed by collisions with atomic hydrogen, and so it is conceivable that enough could survive in high-density primordial gas to render it the dominant coolant. It is this possibility that the present paper examines.

In §2, we briefly outline the numerical method used in this investigation, and in §3 we present results from several simulations which examine the basic effectiveness of H_3^+ cooling and quantify its sensitivity to the values adopted for two key parameters: the critical density for H_3^+ cooling and the strength of the ionizing background. We conclude in §4 with a brief discussion and an outline of future work.

2. Numerical method

The chemical and thermal evolution of gravitationally collapsing primordial gas were investigated using a one-zone model, in which the gas density was assumed to evolve as

$$\frac{d\rho}{dt} = \frac{\rho}{t_{\text{ff}}}, \quad (2.1)$$

where $t_{\text{ff}} = \sqrt{3\pi/32G\rho}$ is the free-fall time-scale of the gas.

The chemistry of the gas was modelled with an extensive chemical network, consisting of 162 reactions among 23 atomic and molecular species. This network includes terms corresponding to ionization by a flux of hard X-ray photons or high-energy cosmic rays. To quantify these rates, it is sufficient to specify the ionization rate of atomic hydrogen, ζ_{H} , which we treat as a free parameter. Full details of this network, including a critical discussion of the rate coefficients used for several key reactions, are given elsewhere.

The thermal evolution of the gas was followed using a cooling function that included contributions from H_2 rotational and vibrational emission (Le Bourlot *et al.* 1999), H_2 collision-induced emission¹ (Ripamonti & Abel 2004) and H_3^+ rotational and vibrational emission, modelled as described later. The coupled set of chemical rate equations was solved implicitly, together with the energy equation, by use of the DVODE solver (Brown *et al.* 1989).

The primordial elemental abundances used in the simulations were taken from Cyburt (2004) and the initial chemical abundances came from Stancil *et al.* (1998). The simulations presented in this paper were run with an initial density $n_{\text{i}} = 1 \text{ cm}^{-3}$ and an initial temperature $T_{\text{i}} = 1000 \text{ K}$, but the results at the densities of interest are insensitive to these choices. The simulations were terminated after $t = 2.748 \times 10^{15} \text{ s}$, once the density reached $n_{\text{f}} = 10^{14} \text{ cm}^{-3}$, as at densities higher than this H_2 collision-induced emission becomes the dominant

¹ This is the inverse process of the more commonly known collision-induced absorption process.

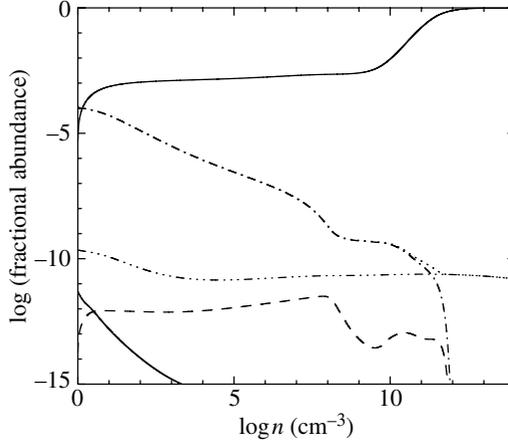


Figure 1. Evolution of the fractional abundances of H_2 (upper solid line), H_3^+ (dashed line), H^+ (dash-dotted line), e^- (dotted line), Li^+ (dash-dot-dot-dotted line) and H_2^+ (lower solid line) as a function of gas number density n in our standard run.

cooling process. As we show in §2a, very little H_3^+ remains in the gas by the time it reaches this density.

Our simulations were run with an initial redshift $z=20$, but the results are not sensitive to this choice.

(a) H_3^+ cooling

At gas densities where the H_3^+ level populations are in LTE, the effects of H_3^+ cooling are straightforward to treat using the LTE cooling rate of Neale *et al.* (1996). At densities where H_3^+ is not in LTE, however, any accurate determination of the cooling rate requires knowledge of the rate at which excited levels of H_3^+ are populated by collisions between H_3^+ and H or H_2 , and this information is not presently available. Therefore, in this preliminary investigation, H_3^+ cooling has been modelled in an extremely simple fashion. We have approximated the H_3^+ cooling function as

$$A_{H_3^+} = A_{LTE,H_3^+} \times \min \left[1, \frac{n}{n_{cr,H_3^+}} \right], \tag{2.2}$$

where A_{LTE,H_3^+} is the LTE cooling rate, and where we treat the critical density n_{cr,H_3^+} as an adjustable parameter. We can estimate n_{cr,H_3^+} by noting that radiative de-excitation rates from excited vibrational states of H_3^+ are typically approximately 10^2 s^{-1} , while collisional excitation rates for collisions with H or H_2 are unlikely to be larger than $10^{-9} \text{ cm}^3 \text{ s}^{-1}$, and may be much smaller. This implies that $n_{cr,H_3^+} \geq 10^{11} \text{ cm}^{-3}$. We chose $n_{cr,H_3^+} = 10^{11} \text{ cm}^{-3}$ as a default value for our simulations, but also explored the effects of varying n_{cr,H_3^+} .

3. Results

In figure 1, we show how the abundances of H_2 , H^+ , H_2^+ , H_3^+ , Li^+ and electrons vary during the course of what we consider to be our standard run: a simulation in which we set $n_{cr,H_3^+} = 10^{11} \text{ cm}^{-3}$ and $\zeta_H=0.0$. At densities $n < 10^8 \text{ cm}^{-3}$, the

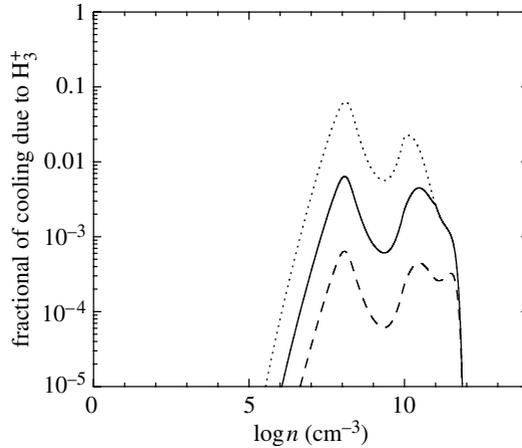


Figure 2. Contribution of H_3^+ to the total cooling rate, plotted for runs in which $n_{\text{cr},\text{H}_3^+} = 10^{11} \text{ cm}^{-3}$ (solid line), 10^{12} cm^{-3} (dashed line) and 10^{10} cm^{-3} (dotted line).

evolution of the H_3^+ abundance closely tracks that of the H_2 abundance, with $x_{\text{H}_3^+}/x_{\text{H}_2} \sim 10^{-9}$. In this regime, the low H_2^+ abundance means that little H_3^+ is produced by the reaction



which is the dominant source of H_3^+ in the Galactic interstellar medium. Instead, the main source of H_3^+ is the radiative association of H^+ with H_2 ,



The rate coefficient that we adopted for this reaction is $k_{\text{ra}} = 10^{-16} \text{ cm}^3 \text{ s}^{-1}$, which is consistent with the value measured by Gerlich & Horning (1992). The main destruction mechanism in this regime is dissociative recombination



for which we use the rate coefficient of McCall *et al.* (2004). As $x_{\text{H}^+} \simeq x_{\text{e}}$, the H_3^+ abundance that results from the balance between these two reactions is independent of the fractional ionization. However, it should be noted that the H_3^+ abundance in this regime is sensitive to the value of the rate coefficient for reaction (3.2), which is highly uncertain (Flower & Pineau des Forêts 2003).

At densities $n > 10^8 \text{ cm}^{-3}$, the H_3^+ abundance begins to decrease, because compressional and chemical heating, whose effects are not fully offset by radiative cooling, cause the gas to become warm enough for the endothermic reaction



to operate. The rising H_2 abundance at $n > 10^9 \text{ cm}^{-3}$ leads to increased production of H_3^+ through reaction (3.2) and so offsets this reduction for a while, but eventually both the H^+ and the H_3^+ abundances fall-off sharply as the time-scale for their removal from the gas becomes shorter than the free-fall collapse time-scale. For $n > 10^{12} \text{ cm}^{-3}$, the most abundant positive ion in the gas is Li^+ , and at these densities, very little H^+ or H_3^+ remains.

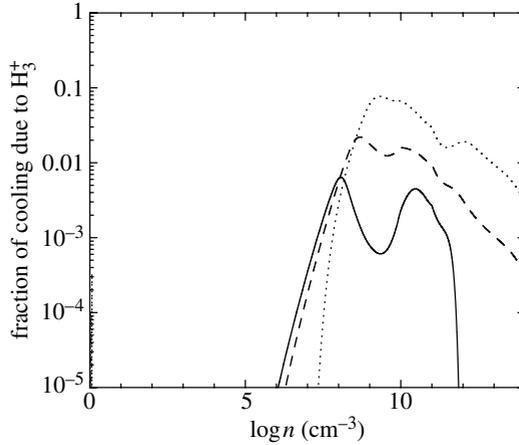


Figure 3. Contribution of H_3^+ to the total cooling rate, plotted for runs in which the ionization rate $\zeta_H=0.0$ (solid line), 10^{-19} s^{-1} (dashed line) and 10^{-18} s^{-1} (dotted line).

In figure 2, we show what fraction of the total cooling is produced by H_3^+ . At low densities ($n < 10^7 \text{ cm}^{-3}$), H_2 is still an effective coolant and the contribution from H_3^+ is negligible. For densities $10^7 < n < 10^{12} \text{ cm}^{-3}$, H_3^+ does become marginally important, but never contributes more than about 0.6% of the total cooling. Finally, at $n > 10^{12} \text{ cm}^{-3}$, cooling from H_3^+ again becomes negligible, owing to the sharp fall-off in the H_3^+ abundance at these densities.

Figure 2 also indicates how the influence of H_3^+ cooling varies as we vary n_{cr,H_3^+} . In our treatment, an increase in n_{cr,H_3^+} is equivalent to a decrease in the low-density H_3^+ cooling rate, and we see from figure 2 that an increase in n_{cr,H_3^+} of an order of magnitude leads to an order of magnitude decrease in the contribution from H_3^+ to the total cooling rate and vice versa. If we were to decrease n_{cr,H_3^+} by a factor of a hundred or more, then this would be enough to make H_3^+ the dominant coolant at densities between 10^7 and 10^{12} cm^{-3} . As noted earlier, we consider this to be highly unlikely, and expect that $n_{\text{cr},H_3^+} \geq 10^{11} \text{ cm}^{-3}$, but a definitive conclusion on this point will require better modelling of H_3^+ cooling, together with better atomic and molecular data.

The influence of an ionizing background in the form of hard X-rays or cosmic rays is explored in figure 3. We plot the contribution to the total cooling rate made by H_3^+ in three different models: our standard model, as described earlier, together with two other models with $\zeta_H = 10^{-19}$ and 10^{-18} s^{-1} . As we increase ζ_H , the contribution of H_3^+ to the cooling rate also increases. This is owing to the production of H_2^+ ions from H_2 by the ionizing flux, some fraction of which then form H_3^+ via reaction (3.1). We see from figure 3 that if the ionization rate is larger than 10^{-18} s^{-1} , then the contribution from H_3^+ to the total cooling rate will be significant; indeed, if ζ_H is large enough, then H_3^+ cooling may even dominate.

Is it physically plausible for there to be an ionization rate as large as this in dense primordial gas? This depends on the assumption that we make about the source of the ionization. To produce an ionization rate $\zeta_H \sim 10^{-18} \text{ s}^{-1}$, we would require an energy density in hard X-rays of roughly $10^{-14} \text{ erg cm}^{-3}$, or an energy density in 100 MeV cosmic rays of a similar order of magnitude. These values are much larger than could reasonably be produced as extragalactic

backgrounds, even with the most optimistic assumptions, but may be plausible if there are sources of hard X-rays or cosmic rays close to the collapsing gas.

4. Discussion

The simple models presented in this paper demonstrate that H_3^+ cooling is unlikely to be of major importance in dense primordial gas, unless a significant ionizing flux of hard X-rays or cosmic rays is also present. However, this conclusion is sensitive to the details of our approximate treatment of non-LTE H_3^+ cooling and may also be sensitive to some of the other simplifications in our present model. We are presently addressing these issues by performing a parameter study that examines a much wider range of models, and that uses a more detailed treatment of non-LTE H_3^+ cooling, based on the approach of Oka & Epp (2004). We hope to report results from these simulations in the near future.

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