Primordial molecular clouds

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Abstract. It is now well known that a primordial chemistry, involving light elements produced during the nucleosynthesis period, might develop during the hydrogen post-recombination era. In particular, molecular ions and primordial molecules such as \( \text{H}_2 \), HD and LiH will be produced. We summarize this primordial chemistry after the recombination epoch, and then present a simple gravitational collapse model of a cloud. The potentiality of fragmentation of this collapsing protoclouds through the thermal instability is also discussed. We suggest that this study could also be extended to the CO molecule, because the carbon reservoir molecule CO has already been observed in high redshifts objects.

I INTRODUCTION

The study of primordial chemistry of molecules addresses a number of interesting questions pertaining to the thermal balance of collapsing molecular protoclouds. In numerous astrophysical cases molecular cooling and heating influence dynamical evolution of the medium, see for example the review done by Dalgarno and McCray (1972) who present molecular cooling and heating in HI regions, or Shu (1997) who discusses the influence of molecules in star formation.

The existence of a significant abundance of molecules can be crucial on the dynamical evolution of collapsing objects. Because the cloud temperature increases with contraction, a cooling mechanism can be important for the structure formation, by lowering pressure opposing gravity, i.e. by allowing continued collapse of Jeans unstable protoclouds. This is particularly true for the first generation of objects. Many authors have examined this problem (Bodenheimer 1968, Hutchins 1976, Palla et al 1983, Villere & Bodenheimer 1987, Tegmark et al 1997) introducing molecular coolants, mainly \( \text{H}_2 \) molecules. From Fall and Rees (1985) we know that \( \text{H}_2 \) molecules are important cooling agents and can lead, sometimes, to the fragmentation process of the object and thus provide a possible scenario of globular cluster formation for collapsing galaxies.

Recently Puy and Signore (1997), Bougleux and Galli (1997) showed that during the early stages of gravitational collapse, for some collapsing masses, HD molecules were the main cooling agent when the collapsing protostructure had a temperature of about 200 Kelvins. In our last papers (Puy and Signore 1997, 1998) we have numerically calculated the cooling functions for \( \text{H}_2 \), HD and LiH molecules by considering the excitation of the twenty first rotational levels. \( \text{H}_2 \) is an homonuclear molecule, so radiative transitions within the lowest electronic state involve only quadrupole transitions, \( \Delta J = 2 \). Between two rotational levels, \( \Delta J = J + 2 - J \) the energy of the transition is given by

\[
E_{J+2,J} = 2kB_r(2J + 3) = kT_{J+2,J}
\]

where \( T_{J+2,J} \) is the temperature of the quadrupolar transition \( J + 2 \rightarrow J \), \( B_r \) the rotational constant (for \( \text{H}_2 \), \( B_r = 85.33 \) Kelvins) and \( k \) the Boltzmann constant. Due to the non-zero dipole moment the transitions involve dipolar transitions, \( \Delta J = 1 \). Thus the energy of the transition \( J \rightarrow J + 1 \) is given by:

\[
E_{J+1,J} = 2kB_r(J + 1) = kT_{J+1,J}
\]

\( T_{J+1,J} \) is the temperature of the dipolar transition \( J + 1 \rightarrow J \), \( B_r = 64.3 \) Kelvins for HD and \( B_r = 10.7 \) Kelvins for LiH.

In this paper we consider a collapsing molecular protocloud made up only of \( \text{H}_2 \) and HD molecules. We do not consider collisions with H atoms because we consider only the central part of the cloud where the molecules are
present. In this picture $H$ is less heavier and is confined in the circumcloud. Moreover, we do not consider the evolution of abundances. Puy & Signore (1998) showed that the evolution of $H_2$ and $HD$ abundance was low, and abundance of $LiH$ was negligible (see also Stancil et al. 1996). Thus, the constant ratio $\eta = n_{H_2}/n_{HD}$ (where $n_{H_2}$ and $n_{HD}$ are respectively the density of $H_2$ and the density of $HD$) around the primordial ratio

$$\eta_{\text{prim.}} = n_{H_2}/n_{HD} \sim 1430$$

(in the framework of the Standard Big Bang nucleosynthesis, see Puy et al 1993).

In section 2, we recall the primordial chemistry. In section 3, with these approximations, we analytically calculate the population of the ground state level and first state level in order to evaluate the molecular cooling and molecular heating due to $HD$ and $H_2$ molecules. In section 4, we estimate the molecular cooling during the collapse of protoclouds. Then, in section 5, the possibility of thermal instability during the early phase of gravitational collapse is discussed. Finally, in section 6, we suggest that this study could be extended to $CO$ molecules which have been recently detected at redshifts $z > 4$ (Ohta et al 1996, Omont et al 1996, Guilloteau et al 1997).

### II PRIMORDIAL CHEMISTRY

In standard Big Bang theory, chemistry took place around the epoch of recombination. At $z \sim 1000$ the chemical species essentially were (see Signore & Puy 1999):

$$H, H^+, D, D^+, He, Li$$

As the Universe expanded and cooled, different routes led to molecular formation. Many authors have described in detail primordial molecular formation and evolution; in particular, Puy et al. (1993) have simultaneously solved the coupled chemical equations and the density and temperature evolution equations. Finally with initial conditions given by the Standard Big Bang Nucleosynthesis (Signore & Puy 1999), we obtain the following abundances (see Puy & Signore 1999):

$$H_2/H \sim 8.4 \times 10^{-5}$$

$$HD/H \sim 10^{-5}$$

$$LiH/H \sim 10^{-17}$$

In the following due to the very low abundance of $LiH$ we will consider only the primordial molecules $H_2$ and $HD$.

### III ANALYTIC CALCULATIONS OF COOLING AND HEATING FUNCTIONS OF $H_2$ AND $HD$ MOLECULES

We consider here only the transition between the ground state and the first state. Due to the existence of a permanent dipolar moment for $HD$ ($\mu_{HD} = 8.3 \times 10^{-4}$ Debye, Abgrall et al 1982), the transition concerning $HD$ molecule is a dipolar transition whereas for $H_2$ molecule the transition is quadrupolar (because it has no permanent dipolar moment).

#### A HD molecule

The excitation of the ground state is radiative or collisional, the equations of evolution concerning the populations ($X_o^{HD}$ for the ground state $J = 0$, $X_1^{HD}$ for the first excited state $J = 1$) are given by:

$$\frac{dX_o^{HD}}{dt} = \left[C_{0,1}^{HD} + B_{0,1}^{HD} u_{0,1}^{HD}\right] X_o^{HD} - \left[A_{0,1}^{HD} + C_{1,0}^{HD} + B_{1,0}^{HD} u_{1,0}^{HD}\right] X_1^{HD}$$

$$\frac{dX_1^{HD}}{dt} = \left[A_{1,0}^{HD} + C_{1,0}^{HD} + B_{1,0}^{HD} u_{1,0}^{HD}\right] X_1^{HD} - \left[C_{0,1}^{HD} + B_{0,1}^{HD} u_{0,1}^{HD}\right] X_o^{HD}$$
where \( C_{0,1}^{HD} \) and \( C_{1,0}^{HD} \) are the collisional coefficients characterizing the collisions between \( HD \) and \( H_2 \). In the approximation of Maxwell-Boltzmann distribution we have:

\[
C_{0,1}^{HD} = 3C_{1,0}^{HD} \exp \left( -\frac{T_{0,1}^{HD}}{T_m} \right)
\]

with \( T_{0,1}^{HD} = T_{0,1}^{HD} \) the transition temperature between \( J = 0 \to J = 1 \), \( T_m \) the temperature of the matter inside the collapsing cloud, \( B_{0,1}^{HD} \) and \( B_{1,0}^{HD} \) are the Einstein coefficients. The radiative density is

\[
u_1^{HD} = \nu_{0,1}^{HD} = \frac{8\pi h(\nu_{20}^{HD})^3}{c^3} \frac{1}{\exp\left(\frac{T_{0,1}^{HD}}{T}\right) - 1}
\]

where \( \nu_{0,1}^{HD} \) and \( T_{0,1}^{HD} \) are the corresponding frequency and temperature, \( h \) the Planck constant, \( c \) the velocity of the light and \( T_r \) the temperature of the background radiation.

\[
A_{1,0}^{HD} = \frac{512 \pi^4 k^3}{3h^3 c^3} \frac{B_{0,1}^{HD} \nu_{20}^{HD}^2}{3}
\]

characterizes the Einstein coefficient for the spontaneous emission (see Kutner 1984) and \( B_{HD} = 64.3 \) Kelvins the rotational constant (see Herzberg 1950).

We have the following normalisation for the populations:

\[
X_o^{HD} + X_1^{HD} = 1
\]

Moreover we consider a quasi-instantaneous transition so

\[
\frac{dX_o^{HD}}{dt} = \frac{dX_1^{HD}}{dt} = 0
\]

Thus from these approximations we find for the populations \( X_1^{HD} \) and \( X_o^{HD} \):

\[
X_1^{HD} = \frac{A_{1,0}^{HD} u_{0,1}^{HD} + C_{1,0}^{HD}}{A_{1,0}^{HD} u_{0,1}^{HD} + u_{0,1}^{HD} (B_{0,1}^{HD} + B_{1,0}^{HD}) + C_{0,1}^{HD} + C_{1,0}^{HD}}
\]

and

\[
X_o^{HD} = \frac{A_{1,0}^{HD} B_{1,0}^{HD} u_{1,0}^{HD} + C_{1,0}^{HD}}{A_{1,0}^{HD} u_{0,1}^{HD} (B_{0,1}^{HD} + B_{1,0}^{HD}) + C_{0,1}^{HD} + C_{1,0}^{HD}}
\]

The probability of collisional de-excitation is given by

\[
P_{c}^{HD} = \frac{C_{1,0}^{HD}}{C_{1,0}^{HD} + A_{1,0}^{HD} + B_{1,0}^{HD} u_{1,0}^{HD}}
\]

and the probability of radiative de-excitation:

\[
P_{r}^{HD} = \frac{A_{1,0}^{HD} + B_{1,0}^{HD} u_{1,0}^{HD}}{C_{1,0}^{HD} + A_{1,0}^{HD} + B_{1,0}^{HD} u_{1,0}^{HD}}
\]

Thus, we can calculate the molecular cooling (collisional excitation followed by a radiative de-excitation):

\[
\Lambda_{HD} = n_{HD} X_o^{HD} C_{0,1}^{HD} P_r^{HD} E_{1,0}^{HD}
\]

where \( E_{1,0}^{HD} = kT_{1,0}^{HD} \) is the energy for the transition \( J = 0 \to J = 1 \).

The molecular heating (radiative excitation followed by collisional de-excitation) is:

\[
\Gamma_{HD} = n_{HD} X_o B_{0,1}^{HD} C_{0,1}^{HD} P_c^{HD} E_{1,0}^{HD}
\]

If we take into account the following relation between the Einstein coefficients:

\[
P_{0,1}^{HD} = 3B_{1,0}^{HD} \quad \text{and} \quad B_{1,0}^{HD} = \frac{c^3}{8\pi h(\nu_{20}^{HD})^3} A_{1,0}^{HD}
\]
then we deduce for the molecular cooling

$$\Lambda_{HD} = \frac{3C_{1,0}^{HD} \exp(-\frac{T_{1,0}^{HD}}{m_T}) \exp\left(\frac{T_{1,0}^{HD}}{m_T}\right) h\nu_{1,0}^{HD} n_{HD} A_{1,0}^{HD}}{A_{1,0}^{HD} \left[3 + \exp\left(\frac{T_{1,0}^{HD}}{m_T}\right)\right] + C_{1,0}^{HD} \left[1 + 3\exp(-\frac{T_{1,0}^{HD}}{m_T})\right] \exp\left(\frac{T_{1,0}^{HD}}{m_T}\right) - 1}$$ (11)

and for the molecular heating

$$\Gamma_{HD} = \frac{3C_{1,0}^{HD} h\nu_{1,0}^{HD} n_{HD} A_{1,0}^{HD}}{A_{1,0}^{HD} \left[3 + \exp\left(\frac{T_{1,0}^{HD}}{m_T}\right)\right] + C_{1,0}^{HD} \left[1 + 3\exp(-\frac{T_{1,0}^{HD}}{m_T})\right] \exp\left(\frac{T_{1,0}^{HD}}{m_T}\right) - 1}$$ (12)

Notice that calculating the ratio molecular cooling to molecular heating we obtain the following simple expression

$$\eta_{HD} = \frac{\Lambda_{HD}}{\Gamma_{HD}} = \exp\left(\frac{T_{1,0}^{HD} (T_m - T_r)}{T_r T_m}\right)$$ (13)

This relation gives us an important information concerning the thermal influence of the thermal function $\Psi_{HD} = \Gamma_{HD} - \Lambda_{HD}$ during a gravitational collapse. When the matter temperature $T_m$ is higher than the radiative temperature, we have $\eta_{HD} > 1$, i.e. $\Lambda_{HD} > \Gamma_{HD}$ so molecules cool the collapsing cloud. Thus during a gravitational collapse, the matter temperature of the collapsing cloud is higher than the radiative temperature of the cosmological background (let us recall that in our case we do not consider some external sources like quasars, first stars etc...).

Thus in this study, we consider only the molecular cooling which is the dominant term in the cooling function as we have shown for a collapsing cloud (Puy & Signore 1996). Moreover if we compare the temperature of the dipolar transition for $HD$, $J = 0 \rightarrow J = 1$, $T_{10}^{HD} = 128.6$ K with the temperature of the cosmological radiation between the redshifts $[5, 20]$, i.e. $T_r \in [13.5, 54]$, we can approximate:

$$3 + \exp\left(\frac{T_{10}^{HD}}{T_r}\right) \sim \exp\left(\frac{T_{10}^{HD}}{T_r}\right)$$

and

$$\exp\left(\frac{T_{10}^{HD}}{T_r}\right) - 1 \sim \exp\left(\frac{T_{10}^{HD}}{T_r}\right)$$

Therefore, with these approximations, we obtain for the cooling function of $HD$ (Eq. 9) the expression:

$$\Lambda_{HD} \sim \frac{3C_{1,0}^{HD} \exp(-\frac{T_{1,0}^{HD}}{m_T}) h\nu_{1,0}^{HD} n_{HD} A_{1,0}^{HD}}{A_{1,0}^{HD} + C_{1,0}^{HD} \left[1 + 3\exp(-\frac{T_{1,0}^{HD}}{m_T})\right]}$$ (14)

### B $H_2$ molecule

Concerning the $H_2$ molecules, the analysis is the same than that for the $HD$ molecules with the difference that the studied transitions are quadrupolar. Because of the increased number of charged particle regions with molecules ($H_2$, $HD$...), the heating mechanism is different from and more complicated than that of atomic regions. We focus our calculations only on the first transition $J = 0 \rightarrow J = 2$. The other transitions are negligible because we consider the early phase of gravitational collapse where the matter temperature is below 200 Kelvins which is much lower than the transition temperatures for $H_2$ molecules (see Table 1). The Einstein coefficients for the spontaneous emission and for the first transition are given by (see Kutner 1984):

$$A_{2,0}^{H_2} = 2.44 \times 10^{-11} \text{ s}$$

The relations between the Einstein coefficients are

$$B_{0,2}^{H_2} = 5B_{2,0}^{H_2} \quad \text{and} \quad B_{2,0}^{H_2} = \frac{c^3}{8\pi (\nu^{H_2})^3} A_{2,0}^{H_2}$$
and the radiative density for the transition is:
\[ u_{2,0}^{H_2} = u_{0,2}^{H_2} = \frac{8\pi h(v_{2,0}^{HD})^3}{c^3} \exp\left(\frac{T_{2,0}^{H_2}}{T_r} - 1\right) \]

and for the collisional coefficients in the Maxwell-Boltzmann distribution approximation:
\[ 5C_{2,0}^{H_2} = C_{2,0}^{H_2} \exp\left(\frac{T_{2,0}^{H_2}}{T_m}\right) \]

by analogy with the \( HD \) molecules and with the same levels of approximations
\[ \exp\left(\frac{T_{2,0}^{H_2}}{T_r} - 1\right) \sim \exp\left(\frac{T_{2,0}^{H_2}}{T_r}\right) \]

and
\[ 5 + \exp\left(\frac{T_{2,0}^{H_2}}{T_r}\right) \sim \exp\left(\frac{T_{2,0}^{H_2}}{T_r}\right) \]

Thus, from the Eqs (5) and (6), we find for the populations \( X_0^{H_2} \) and \( X_1^{H_2} \):
\[ X_0^{H_2} \sim \frac{A_{2,0}^{H_2} + C_{2,0}^{H_2}}{A_{2,0}^{H_2} + C_{2,0}^{H_2} \left(1 + \exp\left(\frac{T_{2,0}^{H_2}}{T_m}\right)\right)} \]
\[ X_1^{H_2} \sim \frac{5C_{2,0}^{H_2} \exp\left(\frac{T_{2,0}^{H_2}}{T_m}\right)}{A_{2,0}^{H_2} + C_{2,0}^{H_2} \left(1 + \exp\left(\frac{T_{2,0}^{H_2}}{T_m}\right)\right)} \]

The probability of radiative de-excitation becomes
\[ P_r^{H_2} \sim \frac{A_{2,0}^{H_2}}{A_{2,0}^{H_2} + C_{2,0}^{H_2}} \]

while the molecular cooling for the \( H_2 \) molecule is given by:
\[ \Lambda_{H_2} \sim \frac{5n_{H_2} C_{2,0}^{H_2} A_{2,0}^{H_2} \exp\left(-\frac{T_{2,0}^{H_2}}{T_m}\right)}{A_{2,0}^{H_2} + C_{2,0}^{H_2} \left[1 + 5\exp\left(-\frac{T_{2,0}^{H_2}}{T_m}\right)\right]} \]

### C Collision rates

The collisional coefficients are given by the expressions:
\[ C_{1,0}^{HD} = <\sigma.v_{HD}> n_{H_2} \]  
\[ C_{2,0}^{H_2} = <\sigma.v_{H_2}> n_{H_2} \]

where \( \sigma \sim 1\AA^2 \) is the collisional cross section and \( n_{H_2} \) the density of \( H_2 \); \( v_{HD} \) and \( v_{H_2} \) are respectively the velocity of \( HD \) and \( H_2 \) given by
\[ v_{HD} = v_{H_2} = \sqrt{\frac{3kT_m}{2m_H}} \]

where \( m_H \) is the hydrogen mass. Notice that, in our model, \( H_2 \) molecules are more abundant than \( HD \) molecules, so \( H_2 \) molecules are the main collisional species.
D Total cooling function

The total cooling function is given by

\[ \Lambda_{Total} = \Lambda_{HD} + \Lambda_{H_2} = \Lambda_{HD}(1 + \xi_{H_2}) \] (19)

where

\[ \xi_{H_2} = \frac{\Lambda_{H_2}}{\Lambda_{HD}} \]

is the ratio between the \( H_2 \) and \( HD \) cooling functions. With the help of the numerical values of the Table 1, we deduce:

\[ \Lambda_{HD} \sim 2.66 \times 10^{-21} n_{HD}^2 \exp\left(-\frac{128.6}{T_m}\right) \frac{\sqrt{T_m}}{1 + n_{HD}\sqrt{T_m}[1 + 3\exp(-\frac{128.6}{T_m})]} \] (20)

\[ \Lambda_{H_2} \sim 1.23 \times 10^{-20} n_{HD}^2 \exp\left(-\frac{512}{T_m}\right) \frac{\sqrt{T_m}}{5 \times 10^{-4} + n_{HD}\sqrt{T_m}[1 + 5\exp(-\frac{512}{T_m})]} \] (21)

and for the ratio:

\[ \xi_{H_2} \sim 4.63 e^{-\frac{201.4}{T_m}} \frac{1 + \sqrt{T_m}n_{HD}[1 + 3\exp(-\frac{128.6}{T_m})]}{5 \times 10^{-4} + \sqrt{T_m}n_{HD}[1 + 5\exp(-\frac{512}{T_m})]} \] (22)

IV MOLECULAR FUNCTIONS OF A COLLAPSING PROTOCLOUD

We study a homologous model of spherical collapse of mass \( M \) similar to the model adopted in Lahav (1986) and Puy & Signore (1996) in which we only consider \( H_2 \) and \( HD \) molecules.

We have seen (Puy & Signore 1997) from a numerical integration of the cooling functions where twenty rotational levels were considered that molecular cooling is important. Moreover we have shown that below 200 Kelvins the main cooling agent is the \( HD \) molecule. The aim of this paper is to analyse, through our approximations (where the only two first excited levels are considered), the evolution of the cooling and the potentiality of thermal instability.

First, let us recall the equations governing dynamics of a collapsing protocloud:

\[ \frac{dT_m}{dt} = -2 T_m \frac{dr}{dr} - \frac{2}{3nk} \Lambda_{Total} \] (23)

for the evolution of the matter temperature \( T_m \),

\[ \frac{d^2r}{dt^2} = \frac{5kT_m}{2m_Hr} - \frac{GM}{r^2} \] (24)

for the evolution of the radius \( r \) of the collapsing cloud and

\[ \frac{dn}{dt} = -\frac{3n}{r} \frac{dr}{dt} \] (25)

for the evolution of the matter density \( n \).

At the beginning of the gravitational collapse the matter temperature increases, then due to the very important efficiency of the molecular cooling, the temperature decreases. We consider here this transition regime i.e. the point where the temperature curve has a horizontal asymptot (see Puy & Signore 1997):

\[ \frac{dT_m}{dt} = 0 \]

and where the cooling due to molecules can exceed the heating resulting from the collapse. From the equation (22) of the evolution of the matter temperature, we deduce

\[ -2 \frac{T_m}{r} \frac{dr}{dt} = \frac{2}{3nk} \Lambda_{Total} \]
Note that the total molecular cooling is negative ($\Lambda_{\text{Total}} < 0$). Moreover, because we consider the early phase of the gravitational collapse, we can approximate to a free fall collapse and so the pressure term, $5kT_m/2m_Hr$, is negligible in the equation (23). Thus, the evolution equation of the radius can be written:

$$\frac{d^2r}{dt^2} = -\frac{GM}{r^2}$$

which leads to

$$\frac{dr}{dt} = \frac{GM}{r} \quad (26)$$

Moreover, because we know that the evolution of the density is:

$$n = n_o \left(\frac{r}{r_o}\right)^3 \quad (27)$$

where $n_o$ and $r_o$ are respectively the density and the radius at the beginning of the collapse. Thus we conclude that

$$\Lambda_{\text{Total}} = \frac{3n_o k T_m r_o^3}{r^3} \frac{GM}{r^2} \quad (28)$$

We have seen that the regime of temperature that we consider is below 200 Kelvins. Moreover, the abundances of $HD$ and $H_2$ remain roughly constant during the early phase of the gravitational collapse (Puy & Signore 1997, 1998). In this case, the value of the density of $HD$ at the beginning of the collapse is $n_{HD} \sim 6 \times 10^{-8} \text{ cm}^{-3}$. The temperature of the matter is below 200 Kelvins. Thus we can approximate the following terms as follows:

$$1 + n_{HD} \sqrt{T_m} \left[1 + 3 \exp\left(-\frac{128.6}{T_m}\right)\right] \sim 1$$

$$5 \times 10^{-4} + n_{HD} \sqrt{T_m} \left[1 + 5 \exp\left(-\frac{512}{T_m}\right)\right] \sim 5 \times 10^{-4}$$

These approximations lead to the following simplified expressions for the molecular cooling

$$\Lambda_{HD} \sim \Lambda_o \exp\left(-\frac{T_o}{T_m}\right) n_{HD}^2 \sqrt{T_m} \quad (29)$$

where $\Lambda_o$, $T_o$ and $\Delta T_o$ are constants:

$$\Lambda_o = 2.66 \times 10^{-21} \text{ erg cm}^{-3} \text{ K}^{-1/2} \text{ s}^{-1}$$

$$T_o = T_{1.0}^{HD} = 128.6 \text{ K}$$

$$\Delta T_o = T_{2.0}^{H_2} - T_{1.0}^{HD} = 383.4 \text{ K}$$

From our homologous model of gravitational collapse, the density of matter is the density of the species which is the most abundant so $n = n_{H_2}$ which gives

$$n_{HD} = \frac{n_{H_2}}{\eta_{\text{Prim.}}} = \frac{n}{\eta_{\text{Prim.}}} = \frac{n_o}{\eta_{\text{Prim.}}} \left(\frac{r_o}{r}\right)^3 \quad (30)$$

Finally we find for the total cooling

$$\Lambda_{\text{Total}} \sim \Lambda_o \exp\left(-\frac{T_o}{T_m}\right) \frac{n_o^2 r_o^6}{\eta_{\text{Prim.}}^2 \sqrt{T_m}} \left[1 + \xi_o \exp\left(-\frac{\Delta T_o}{T_m}\right)\right] \quad (31)$$

With $\xi_o = 9260$, if we take for the mass of the cloud the following approximation:

$$M \sim 2m_H n_o r_o^3$$
from equations (28) and (32) we deduce for the the radius

$$r \sim \kappa \frac{\exp(-T_o/T_m)}{\sqrt{T_m}} \left[ 1 + \xi_o \exp(-\Delta T_o/T_m) \right]^{3/2} \quad (32)$$

where the constant

$$\kappa = \frac{\Lambda_o}{6 \hbar^2 k_G \mu_m \kappa} \sim 1.4 \times 10^{22}$$

Finally we obtain for the total molecular cooling

$$\Lambda_{Total} = \delta T_m^{7/2} \frac{\exp(5T_o/T_m)}{\sqrt{T_m}} \left[ 1 + \xi_o \exp(-\Delta T_o/T_m) \right]^{3/2} \quad (33)$$

with

$$\delta = \alpha M^2 \text{ with } \alpha = \frac{3kG}{2m_H \kappa^5}$$

V THERMAL INSTABILITY

We have learned much about thermal instability in the last 30 years since the appearance of the work of Field (1965). Many studies have focused on the problem of thermal instabilitie in different situations: formation of galaxies (Sofue 1969), expanding medium (Kondo 1970), formation of protostars (Stein et al. 1972), formation of globular clusters (Fall & Rees 1985), cooling flows (David et al. 1988) and quasar clouds (Mathews & Doane 1990).

The correct instability criterion can be derived physically as follows. In an infinite, uniform, static medium of density $n_o$ and $T_o$, the continuity and force equations are automatically satisfied. If we introduce a perturbation of density and temperature such that some thermodynamics variable (pressure, temperature...) is held constant, the entropy $S$ will change by an amount $\delta S$, and the heat-loss function, by an amount $\delta \Psi = \Gamma - \Lambda$. From the equation

$$\delta \Psi = -Td(\delta S)$$

there is instability only if:

$$\left( \frac{\delta \Psi}{\delta S} \right) > 0$$

We know that $TdS = C_p dT$ in an isobaric perturbation. The corresponding inequality can be written:

$$\left( \frac{\delta \Psi}{\delta T} \right)_p = \left( \frac{\delta \Psi}{\delta T} \right)_n + \frac{\partial n}{\partial T} \left( \frac{\delta \Psi}{\delta n} \right)_T < 0$$

which characterizes the Field’s criterion. The criterion involves constant $P$ because small blobs tend to maintain pressure equilibrium with their surroundings when heating and cooling get out of balance. In our case (i.e. at the transition regime), a thermal instability could spontaneously be developped if the Field’s Criterion is verified:

$$\frac{\partial \ln \Lambda}{\partial \ln T_m} < 0 \quad (34)$$

In our case the logarithmic differential of the total molecular cooling function is given by

$$\frac{\partial \ln \Lambda}{\partial \ln T_m} = \frac{T_m + 7T_m \xi_o e^{-\Delta T_o/T_m} - 10T_o - 10T_o \xi_o e^{-\Delta T_o/T_m} - 10\xi_o \Delta T_o e^{-\Delta T_o/T_m}}{2 + 2 \xi_o e^{-\Delta T_o/T_m}} \quad (35)$$

Therefore, the criterion is independant of the mass $M$ of the cloud at the transition regime. In figure 1, we have plotted the curve $y(T_m) = \partial \ln \Lambda / \partial \ln T_m$. It shows that the Field’s criterion is always verified.

We conclude that a thermal instability is possible at the transition regime, i.e. at $dT_m/dt = 0$, when cooling (due to molecules) exceeds heating (due essentially to the collapse). Thus by maintaining the same pressure in its surroundings, such a blob would get cooler and cooler and denser and denser until it could separate into miniblobs. This possibility is very interesting and could give a scenario of formation of primordial clouds. However, a quantitative study is necessary to evaluate the order of magnitude of the mass and the size of the clouds. This last point can be crucial particularly concerning the composition of the molecular clouds at high redshift such as the Lyman-\(\alpha\) absorbers in order to evaluate the possible signatures of the primordial clouds.
VI  ON CO MOLECULE

In the very early Universe the components of the primordial molecular medium are formed from the elements of the primordial nucleosynthesis. Later, as soon as stellar processes occur in proto-objects, other molecular species appeared such as CO, CI, HCN. Therefore, their line emission can be seen as an excellent probe of physical conditions of very high redshift objects. Among them, the diatomic molecule CO has the strongest lines at radio wavelengths, the rotational transitions being spaced by 115 GHz in the rest frame at z = 0 (this separation, at a redshift z, becomes compressed by a factor 1/(1 + z)). Moreover, the carbon monoxide line emission had already been detected in four high redshift objects:

1. CO(3 − 2), CO(4 − 3) and CO(6 − 5) in the ultraluminous IR galaxy F10215+4724 at the redshift z = 2.28 (Brown and Van den Bout 1992, Solomon et al 1992).
2. CO(3 − 2), CO(4 − 3), CO(5 − 4) and CO(7 − 6) in the cloverleaf quasar at the redshift z = 2.56 (Barvainis et al 1994, Barvainis et al 1997).
3. CO(5 − 4) in the quasar BR1202-0725 at the redshift z = 4.69 (Ohta et al 1996, Omont et al 1996).
4. CO(5 − 4) in the quasar BRI1335-0418 at the redshift z = 4.41 (Guilloteau et al 1997).

One must also add that, at least for the first three objects, their detectability in molecular transitions may be due to high emissivity of the gas and above all magnification from gravitational lensing rather than an extremely large mass of gas. Moreover, there is no a priori evidence of gravitational lensing for BRI1335-0418. Therefore, if this absence of strong gravitational magnification is confirmed, the fourth object could have a large mass of molecular gas which could be associated with the presence of some huge starburst. However, if there is no doubt about the reality of the CO detection in these objects, it is more difficult to definitively determine the CO to H2 conversion factor in these objects.

Let us also remark that, here, we study protostructures in the mass range 10^8 − 10^{10} M⊙ i.e. in the mass range of dwarf galaxies. Recently, Verter & Hodge (1995) estimated the CO to H2 conversion factor for the very low metallicity dwarf irregular galaxy GR8. They found X > 80 × 10^{20} molecules cm^{-2} (Km s^{-1})^{-1} which is a factor 30 larger than for our Galaxy (X = N(H2)/W_{CO} where N(H2) is the column density of molecular hydrogen gas and W_{CO} is the integration of CO antenna temperature over the velocity profile).

Therefore, from these estimations, the calculations of molecular functions could, in principle, be extended to the CO molecules for collapsing protoclouds at z < 5. The CO molecules could even be a better cooling agent than H2 and HD for some temperature ranges. But, in any case -and in particular for the discussion of thermal instability at the transition regime- the corresponding total cooling function must be numerically calculated because the excitation of many rotational levels must be taken into account. This extended study is beyond the scope of our paper.

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FIGURE 1. $\partial \ln \Lambda_{\text{Total}} / \partial \ln T_m$ in y-axis and temperature of the matter in x-axis (in Kelvins).
REFERENCES

Abgrall H., Roueff E., Viala Y. 1982 A&AS 50, 505
Barvainis R., Tacconi L., Alloin D., Antonucci R., Coleman P. 1994 Nature 371, 586
Barvainis R., Maloney P., Alloin D., Antonucci R. 1997 ApJ 484, 695
Bodenheimer P. 1968 ApJ 153, 483
Bougleux E., Galli D. 1997 MNRAS 288, 638
Brown R. L., Van den Bout P.A. 1992 ApJ 397, L19
Dalgarno A., R.A. Mc Cray 1972, Ann. Rev. Astr. and Ap. 10, 375
David L.P., Bregman J.N., c. Gregory Seab 1988 ApJ 329, 66
Fall S.M., Rees M.J. 1985 ApJ 298, 18
Field G. B. 1965 ApJ 142, 483
Guilloteau S., Omont A., Mc Mahon R.G., Cox P., Petitjean P. 1997 A&A 328, L1
Herzberg G. 1950 in Spectra of diatomic molecules Van Nostrand eds
Hutchins J.B. 1976 ApJ 205, 103
Kondo M. PASJ 22, 13
Kutner M.L. 1984 Fund. Cosm. Phys. 9, 233
Lahu O. 1986 MNRAS 220, 259
Mathews W. G., Doane J. S. 1990 ApJ 352, 423
Ohta K., Yamada T., Nakaniishi K., Kokno K., Akiyama M., Kawabe R. 1996 Nature 382, 426
Omont A., Petitjean P., Guilloteau S., Mc Mahon R.G., Solomon P.M. Pecontal E. 1996 Nature 382, 428
Palla F., Salpeter E.E., Stahler S.W. 1983 ApJ 271, 632
Puy D., Alecian G., Lebourlot J., Léorat J., Pineau des Forêts G. 1993 A&A 267, 337
Puy D., Signore M., 1996, A&A 305, 371
Puy D., Signore M., 1997, New Astron. 2, 299
Puy D., Signore M., 1998, New Astron. 3, 27
Puy D., Signore M., 1999, New Astron. Rev. in press
Shu F.H. 1997 in Molecules in Astrophysics: Probes and Processes pp19, IAU 1997 Van Dishoeck ed.
Sofue Y. 1969 PASJ 21, 211
Solomon P.M., Downes D., Radfort S.J.E. 1992 ApJ 398, L29
Stancil P.C., Lepp S., Dalgarno A. 1996 ApJ 458, 401
Stein R.F., Mc Cray R., Schwarz J. 1972 ApJ 177, L125
Signore M., Puy D., 1999 New Astron. Rev. in press
Tegmark M., Silk J., Rees M.J., Blanchard A., Abel T., Palla F. 1997 ApJ 474,1.
Verter F., Hodge P. 1995 ApJ 446, 616
Villere K. R., Bodenheimer P. in Astrochemistry pp121, IAU 120, eds Vardia, S.P. Tarañdar, Reidel 1987