ON THE POSSIBILITY OF OBSERVING THE DOUBLE EMISSION LINE FEATURE OF H$_2$ and HD FROM PRIMORDIAL MOLECULAR CLOUD CORES

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We study the prospects for observing H$_2$ and HD emission during the assembly of primordial molecular cloud cores. The primordial molecular cloud cores, which resemble those at the present epoch, can emerge around $1 + z \sim 20$ according to recent numerical simulations. A core typically contracts to form the first generation of stars and the contracting core emits H$_2$ and HD line radiation. These lines show a double peak feature. The higher peak is the H$_2$ line of the $J = 2 - 0$ (v=0) rotational transition, and the lower peak is the HD line of the $J = 4 - 3$ (v=0) rotational transition. The ratio of the peaks is about 50, this value characterising the emission from primordial galaxies. The expected emission flux at the redshift of $1 + z \sim 20$ (e.g. $\Omega_m = 0.3$ and $\Omega_\Lambda = 0.7$), in the $J = 2 - 0$ (v=0) line of H$_2$ occurs at a rate $\sim 2 \times 10^{-7}$ Jy; and in the $J = 4 - 3$ (v=0) line of HD at a rate $\sim 4 \times 10^{-9}$ Jy. The former has a frequency of $5.33179 \times 10^{11}$ Hz and the latter is at $5.33388 \times 10^{11}$Hz, respectively. Since the frequency resolution of ALMA is about 40 kHz, the double peak is resolvable. While an individual object is not observable even by ALMA, the expected assembly of primordial star clusters on subgalactic scales can result in fluxes at the 2000-50 $\mu$Jy level. These are marginally observable. The first peak of H$_2$ is produced when the core gas cools due to HD cooling, while the second peak of HD occurs because the medium maintains thermal balance by H$_2$ cooling which must be enhanced by three-body reactions to form H$_2$ itself.

Key words: cosmology: observations — galaxies: formation — ISM: molecules — submillimeter
1. INTRODUCTION

Observation of the first generation of stars presents one of the most exciting challenges in astrophysics and cosmology. Hydrogen molecules (H$_2$s) play an important role as a cooling agent of the gravitationally contracting primordial gas (Saslaw & Zipoy 1967) in the process of primordial star formation. It has been argued that H$_2$ is an effective coolant for the formation of globular clusters (Peebles & Dicke 1969), if such objects precede galaxy formation. The contraction of primordial gas was also studied in the pioneering work of Matsuda, Sato, & Takeda (1969). Thus, we expect the detection of H$_2$ line emission from primordial star-forming regions (Shchekinov 1991). Observational feedback from such Population III objects was examined in Carr, Bond, & Arnett (1984). In the context of the CDM (Cold Dark Matter) scenario for cosmic structure formation, Couchman & Rees (1986) suggested that the feedback from the first structures is not negligible for e.g. the reionisation of the Universe and the Jeans mass at this epoch (e.g. Haiman, Thoul, & Loeb 1996; Gnedin & Ostriker 1997; Ferrara 1998; Susa & Umemura 2000). Recent progress on the role of primordial stars formation in structure formation is reviewed in Nishi et al. (1998) and its future strategy is discussed in Silk (2000).

More recently, the first structures in the Universe have been studied by means of very high resolution numerical simulations (Abel, Bryan, & Norman 2000). The numerical resolution is sufficient to study the formation of the first generation of molecular clouds. According to their results, a molecular cloud emerges with a mass of $\sim 10^5$ solar masses as a result of the merging of small clumps which trace the initial perturbations for cosmic structure formation. Due to the cooling of H$_2$, a small and cold prestellar object appears inside the primordial molecular cloud. It resembles the cores of molecular clouds at the present epoch. These numerical results are consistent with other numerical simulations by Bromm, Coppi, & Larson (1999; 2001). All the simulations predict that the primordial molecular clouds and their cores appear at an epoch of $1 + z \sim 20$ ($z$ is redshift).

According to these results, the first generation of young stellar objects has a mass of $\sim 200$ solar masses, density of $\sim 10^5$ cm$^{-3}$, and temperature of $\sim 200$ K. We stress that these are cloud cores, and not stars. Inside the cores, a very dense structure appears. We call this a kernel for clarity of presentation (Kamaya & Silk 2001). Its density increases to a value as high as $\sim 10^8$ cm$^{-3}$ where three-body reactions for H$_2$ formation occurs. Further evolution is by fragmentation (Palla, Salpeter, & Stahler 1983) and/or collapse (Omukai & Nishi 1998). In the previous paper, we considered the collapsing kernel and the possibility for its observation by future facilities. H$_2$ line emission tracing the temperature structure of
the kernel is potentially detected by ASTRO-F\textsuperscript{1} and ALMA\textsuperscript{2} if the kernels are collectively assembled, as might be expected in a starburst.

Now in the low temperature regime of the typical core, HD is also an important coolant (e.g. Shchekinov 1986). Indeed, Uehara & Inutsuka (1998) show numerically that the core collapses at a relatively low temperature if HD exists. According to them, the primordial filament can reach a temperature of 50 K. Thus, the effect of HD should be examined. Indeed as long as HD is a dominant coolant, it is useful to consider the observational possibility of HD emission from primordial molecular cloud cores, as we do below.

Furthermore, because of the large electric dipole moment, LiH is also potentially an important coolant (Lepp & Shull 1984). Despite the very low abundance of LiH, which means that it is never the dominant coolant, as shown in Lepp & Shull, if its lines are optically thin, it can still be important. We also comment on line cooling by LiH in this paper.

In addition to a contracting primordial cloud, another molecular emission line is discussed by Ciardi & Ferrara (2001) who predict the detection of mid-infrared emission from primordial supernova shell by NGST\textsuperscript{3}. According to Ciardi & Ferrara, the shell can cool and radiate in rotational-vibrational emission lines, and then mid-infrared emission is expected. In particular, the shell can also emit the possible ground rotational line of H\textsubscript{2} (J = 2 − 0 and v = 0). In our first paper, we also predict the primordial emission of the ground rotational line of H\textsubscript{2}. If and when primordial emission of the ground rotational transition is detected, it will be important to judge which is its origin. In this paper, we present a very simple answer to this question.

In §2, we formulate the cooling function for HD and LiH. For H\textsubscript{2}, this was presented in a previous paper (Kamaya & Silk 2001). We summarise the cooling function of H\textsubscript{2} in the Appendix. In §3, we present a model structure for the primordial molecular cloud cores. In §4, we estimate that the luminosity from the cores is primarily due to the emission of H\textsubscript{2}, with a secondary role played by HD, and that LiH is not important. In §5, the observational feasibility of detection is reviewed (differently from the discussion in our previous paper). The theory underlying the observational predictions is presented in §6, and our paper is summarised in the final section.

\textsuperscript{1}http://www.ir.isas.ac.jp/ASTRO-F/index-e.html

\textsuperscript{2}http://www.alma.nrao.edu

\textsuperscript{3}http://ngst.gsfc.nasa.gov
2. DESCRIPTION OF MOLECULAR EMISSION

Primordial molecular cloud cores are expected to be low temperature objects (Abel et al. 2000), where HD (Shchekinov 1986) and LiH (Lepp & Shull 1984) line cooling are frequently considered to be important. In this section, first of all, we present a formalism for the molecular line emission to estimate the luminosity from the cores. The lower rotational transition emission of H$_2$ is also important. Since a detailed description has been presented in the previous paper (Kamaya & Silk 2001), only a brief summary is given in the Appendix.

2.1. HD

HD has a weak electric dipole moment, since the proton in the molecule is more mobile than the deuteron; the electron then does not follow exactly the motion of the positive charge, producing a dipole (Combes & Pfenniger 1997). This moment has been measured in the ground vibrational state from the intensity of the pure rotational spectrum by Trefler & Gush (1968). The measured value is about $5.85 \times 10^{-4}$ Debye ($1 \text{ Debye} = 10^{-18} \text{ in cgs unit}$). Since the first rotational level is about 128 K, the corresponding wavelength is 112 $\mu$m. Since the temperature of the primordial molecular cloud cores (Abel et al. 2000) is about 200 K, HD has sufficient potential to be the dominant coolant (Shchekinov 1986). In this paper, we set the D abundance to be $4 \times 10^{-5}$, keeping consistency for our structural model of cores with their thermal conditions predicted by Uehara & Inutsuka (2000), which is the most recent and detailed analysis for a primordial cloud undergoing HD cooling.

For the cooling function, we adopt the formalism of McKee & Hollenbach (1979). According to this,

$$\Lambda_{\text{HD, thin}} = n \times n_{\text{HD}} \times \frac{4(kT)^2 A_0}{n E_0 (1 + (n_{\text{cr}}/n) + (n_{\text{cr}}/n)^{1.5})} \text{ erg cm}^{-3} \text{ s}^{-1}$$

where $k$ is the Boltzmann constant, $n$ is the gas number density, $n_{\text{cr}}$ is the critical density, $n_{\text{HD}}$ is HD number density, $A_0$ is $3.8 \times 10^{-8} \text{ s}^{-1}$, and $E_0 = 64 k \text{ erg for HD}$. Determining $n_{\text{cr}}$ exactly is a complex calculation, while for our purpose it is sufficient to consider $n_{\text{cr}}$ for the dominant cooling transition if we are interested in the dominant process. Hence, we estimate $n_{\text{cr}}$ via the formalism of McKee & Hollenbach (1979) as $n_{\text{cr}} = 7.7 \times 10^3 \text{ cm}^{-3} (T_g/1000.0)^{0.5}$ where $T_g$ is the thermal temperature of gas.

However, the above formula is inadequate if the temperature is low since the population of the rotationally excited level is small. We consider the cooling function of HD in the optically thin and low temperature regime below 255 K (Galli & Palla 1998) if the density...
is below the critical density for a given temperature;

\[ \Lambda_{\text{HD, n-0}} = 2\gamma_{10}E_{10}\exp\left(-E_{10}/kT_{g}\right) + \left(5/3\right)\gamma_{21}E_{21}\exp\left(-E_{21}/kT_{g}\right). \]  

(2)

Here, \( E_{10} = 128k \text{ erg} \), \( E_{21} = 255k \text{ erg} \), \( \gamma_{10} = 4.410^{-12} + 3.610^{-13}T_{g}^{0.77} \text{ cm}^3 \text{ s}^{-1} \), and \( \gamma_{21} = 4.110^{-12} + 2.110^{-13}T_{g}^{0.92} \text{ cm}^3 \text{ s}^{-1} \). If the gas density is above the critical density, we simply estimate the cooling function by two methods. The first is for the temperature range from 128 K to 255 K. In this range, we simply use Eq.(1) multiplied by \( \exp(-256K/T_{g}) \). This is because the population of \( J = 2 \) to that of \( J = 1 \) is reduced by the factor of \( \exp(256K/T_{g}) \). The second is for if the temperature is below 128 K. In such low temperature case, as simple modification as for the first method for correction is not applicable. Fortunately, the two-level system is a good approximation. Then, we estimate the cooling function from the spontaneous de-excitation rate \( (A) \) of the most probable rotational level of \( J = 1 \) and the collisional de-excitation rate. The de-excitation rate is estimated from the collisional cross section of de-excitation divided by a sound speed. The collisional cross section of de-excitation is typically \( 2.0 \times 10^{-16} \text{ cm}^2 \) for HD (Schaefer 1990). Our approximation breaks at the outer edge of the core, where we smoothly extrapolate keeping the thermal balance. Fortunately, this correction does not alter the main conclusion and the dominant cooling level of \( J \).

On the other hand, to find the cooling function in the optically thick regime, we always need the Einstein A coefficient. We calculate it approximately in the standard way. The coefficient is

\[ A_{J'J} = \frac{64\pi^4\nu_{J'J}^3}{3hc^3}D^2 \frac{J}{2J+1} \]  

(3)

where \( \nu_{J'J} \) is the frequency of the \( J' \rightarrow J \) transition, \( h \) the Planck constant, \( c \) the light speed, \( D \) the electric dipole moment, and \( J \) the rotational quantum number. The results via Eq.(3) describe the exact values of Abgrall et al. (1982) for HD very well.

Once \( J_d(T(r)) \) which is the dominant cooling level of \( J \) is determined at each position of the core, we can modify the optically thin cooling function to the optically thick cooling function by multiplication of the escape probability, \( \epsilon \). To obtain the cooling function for the thick case, hence we define:

\[ \epsilon_{\nu_{J'J}} = \frac{1 - \exp(\tau_{\nu_{J'J}})}{\tau_{\nu_{J'J}}} \]  

(4)

and

\[ \tau_{\nu_{J'J}} = \frac{A_{J'J}c^3}{8\pi\nu_{J'J}^2} \left( \frac{g_{J'}g_J}{g_J - n_J} \right) n_J^2 R_J \delta v \]  

(5)

where \( R_J \) is the Jeans length, \( \delta v \) is the velocity dispersion, and \( g_J \) the statistical weight of \( 2J + 1 \). The velocity dispersion corresponds to Doppler broadening, and is estimated to be
given by the sound speed. The inferred optically thick cooling function is then

\[ \Lambda_{HD, \text{thick}} \equiv \Lambda_{HD, \text{thin}} \times \epsilon_{\nu, j}. \]  

(6)

The procedure of Jeans length shielding in (5) is useful for a simple analytical analysis (Low & Lynden-Bell 1976; Silk 1977).

### 2.2. LiH

The LiH molecule has a much larger dipole moment of 5.9 Debye and the first rotational level is only at 21 K. Thus, although its abundance is very small (\( \sim 10^{-10} \); we adopt this value), there is a plenty of possibility for LiH to be an important coolant (Lepp & Shull 1984). For LiH, fortunately, the formalism of McKee & Hollenbach (1979) is a very good approximation. Then, we use Eq.(1) with parameters for LiH in the thin regime, and the escape probability correction is applied if the optical depth of the dominant line emission is above unity. The adopted parameters are \( A_0 = 0.0113 \text{ s}^{-1} \) and \( E_0/k = 21.0 \text{ K} \), and \( n_{\text{LiH}} \) instead of \( n_{\text{HD}} \). For the corresponding de-excitation rates, we use the results of detailed balance analysis (Bougleux & Galli 1997). The expected collisional de-excitation cross section is found to be approximately \( 5.6 \times 10^{-16} \text{ cm}^2 \), then the de-excitation rate becomes \( 2 \times 10^{-10} \text{ cm}^3 \text{ s}^{-1} \) at \( T_g = 3000 \text{ K} \). Since the de-excitation cross sections tend to be nearly constant at low energies for collisions with neutral particles, the approximate de-excitation rate at lower temperature can be obtained multiplied by the factor of \( (T_g/3000 \text{ K})^{0.5} \). If the comparison with the case of collision of He are interested, the reduced factor of \( 3^{0.5} \) is adopted to account for the difference in the reduced mass (Bougleux & Galli 1997). Their appendix B is useful for further details. If only the optically thin cooling function is needed, appendix A.3 of Galli & Palla (1998) is useful as long as the gas density is below any critical density.

### 3. STRUCTURAL MODEL OF PRIMORDIAL MOLECULAR CLOUD CORE

According to recent numerical simulations, molecular cloud cores appear prior to the formation of population III objects. Cores contain a dense and cool kernel. In our previous paper, we consider how much the kernel emits H\(_2\) line luminosity. In the current paper, we consider the case of the cores. Since the cores have lower temperature than the kernels (e.g. Uehara & Inutsuka 2000), HD and LiH must be considered.

The emission properties are determined by the density and temperature structure of the cores. Fortunately, a reasonably simple model is possible according to Uehara & Inutsuka
We find a fitting formula for the distribution of $H_2$ and temperature which is found by trial and error to approximately reach thermal equilibrium (see the next section). For $f_2(r)$ (solid line in Fig.1):

$$f_2(r) = 0.0001 + 0.495 \times \frac{\exp \left( \frac{n(r)}{10^{11}\text{cm}^{-3}} \right) - \exp \left( \frac{n(r)}{10^{11}\text{cm}^{-3}} \right)}{\exp \left( \frac{n(r)}{10^{11}\text{cm}^{-3}} \right) + \exp \left( \frac{n(r)}{10^{11}\text{cm}^{-3}} \right)} \quad (8)$$

where $n(r) = 10.0^8\text{cm}^{-3}(r/0.01\text{ pc})^{-2.2}$ (the maximum of $f_2(r)$ is set to be 0.5 by definition). This describes approximately the effect of the three body reaction to form $H_2$. For $T(r)$ (dashed line in Fig.1):

$$T(r) = 50 \text{ K} \left( \frac{n(r)}{10^{4.0}\text{cm}^{-3}} \right)^{\frac{1}{2}} \quad (9)$$

We hypothesise that all D and Li are in molecular form above a density of $10^4 \text{ cm}^{-3}$. This is partially supported by Uehara & Inutsuka (2000).

To examine the total emission energy, we need to determine the mass distribution around the centre of the core, where the first star emerges. Also, we assume a spherical configuration for the mass distribution. According to Omukai & Nishi (1998), a high accretion rate is realized if a similarity collapse occurs with the adiabatic heat ratio of 1.1 (e.g. Suto & Silk 1988). The density distribution is described as

$$\frac{\partial \ln \rho(r)}{\partial \ln r} = \frac{-2}{2 - \gamma} \quad (8)$$

Here, $r$ is the radial distance from the centre, $\rho(r)$ is the mass density of atomic H, $H_2$ and He, and $\gamma$ is the specific heat ratio. We set the mass-density distribution of a protostellar-core with $\gamma = 1.1$ as $\rho(r) = \rho_0(r/r_0)^{-2.2}$ where $\rho_0$ is $2.0 \times 10^{-20} \text{ g cm}^{-3}$ and $r_0$ is 0.63 pc. These values are appropriate for fitting a typical protostellar core of Abel et al. (2000).

4. MOLECULE EMISSION LUMINOSITY

We are interested in the dominant rotational emission, then we calculate

$$J_{\text{max}} = \frac{\int_{\text{kernel}} 4\pi r^2 \Lambda_i,\text{thick}(r) J_d(T(r)) dr}{\int_{\text{kernel}} 4\pi r^2 \Lambda_i,\text{thick}(r) dr} \quad (10)$$

Here, for HD ($i=\text{HD}$)

$$J_d(T(r)) = J_d,\text{HD}(T(r)) \equiv \left( \frac{7}{2} \times \frac{T(r)}{64.0 \text{ K}} \right)^{0.5} \quad (11)$$
and for LiH ($i=\text{LiH}$)

$$J_d(T(r)) = J_{d,\text{LiH}}(T(r)) \equiv \left(\frac{7}{2} \times \frac{T(r)}{21.0 \text{ K}}\right)^{0.5},$$

(12)

and for $\text{H}_2$ ($i=\text{H}_2$)

$$J_d(T(r)) = J_{d,\text{H}_2}(T(r)) \equiv \left(\frac{7}{2} \times \frac{T(r)}{85.0 \text{ K}}\right)^{0.5}.$$  

(13)

Here, all $J_d(T(r))$ mean the dominantly contributing $J$-level to the statistical weight at temperature of $T(r)$ (Silk 1983). Using our fitting formula of $f_2(r)$ and $T(r)$, we find each $J_{\text{max}}$ is about 4.0 for HD, 17.0 for LiH, and 2.3 for $\text{H}_2$, respectively. Then, to estimate the dominant line luminosity of $L_{\text{thick}}$ of Eq.(6), we use $J=4$ for HD, $J=17$ for LiH, and $J=2$ for $\text{H}_2$, respectively. The exceptional treatment (but reviewed in Kamaya & Silk 2001) for $\text{H}_2$ is given in the Appendix, according to which we can discuss $J=2-0$ transition of $\text{H}_2$ independent of any other transition.

The estimated total luminosity for a single core ($\int_{\text{core}} 4\pi r^2 \Lambda_{\text{thick}} dr$), $L_{\text{single}}$, is $4.2 \times 10^{35}$ erg s$^{-1}$. Each component is $4.1 \times 10^{35}$ erg s$^{-1}$ for $\text{H}_2$, $1.1 \times 10^{34}$ erg s$^{-1}$ for HD, and $6.9 \times 10^{30}$ erg s$^{-1}$ for LiH. Here, first of all, we find that the contribution due to LiH is very small. This contradicts the conclusion of Lepp & Shull (1984). Fortunately, the reason is simple. Although Lepp & Shull regarded all LiH lines as optically thin, they are optically thick for our case in the region where LiH would be important as suggested by Lepp & Shull.

The line broadening is estimated to be $\sim \delta v_D = (2kT/\mu(r)m_H)^{0.5}$ in the dimension of velocity. Here, $\mu(r)$ is mean molecular weight at each position. Adopting this, the luminosity per Hz (T=1000 K is assumed) is as follows; $\text{H}_2$ rotation emission of $J=2-0$ ($1.1 \times 10^{13}$ Hz; $2.8 \times 10^{-2}$ mm) is $4.0 \times 10^{27}$ erg Hz$^{-1}$, HD rotation emission of $J=4-3$ ($1.1 \times 10^{13}$ Hz; $2.8 \times 10^{-2}$ mm) is $1.0 \times 10^{26}$ erg Hz$^{-1}$, and LiH rotation emission of $J=17-16$ ($7.4 \times 10^{12}$ Hz; $4.0 \times 10^{-2}$ mm) is $9.8 \times 10^{22}$ erg Hz$^{-1}$. Here, we consider the dominant $J_{\text{max}}$ to $J_{\text{max}} - 1$ transitions for HD and LiH, and $J_{\text{max}}$ to $J_{\text{max}} - 2$ transition for $\text{H}_2$.

The total cooling rate at each position is summarised in figure 2. Below $10^8$ cm$^{-3}$, HD is the dominant coolant, while $\text{H}_2$ is dominant above this density. This confirms the results of Lepp and Shull (1984). We also check if our model of the molecular cloud core is reasonable or not. To do it, we estimate the heating rate. In a contracting cloud without dust, the compressional heating is generally dominant. When the three-body reactions for $\text{H}_2$ formation occur, chemical heating is also important. We consider these two heating mechanisms. For compressional heating, we estimate $c_s^2/t_{\text{ff}}$ (e.g. Omukai 2000). The specific free energy for the three-body reaction is 4.48 eV. Our result is displayed in figure 3. The ratio of cooling and heating is given in figure 4. As clearly shown in this figure, the deviation
from the thermal balance is within a factor of three. Thus, our model structure for the core is consistent with thermal balance between molecular line cooling and the expected heating over all of the density range considered in this paper.

5. OBSERVATIONAL FEASIBILITY OF DOUBLE PEAK EMISSION

According to our first paper (Kamaya & Silk 2001), some bright emission lines from assembly of primordial young stellar objects usually have sub-mJy flux as long as the redshift of \( z \) is about 10–40. Then, when we are interested in the same range of the redshift, it is sufficient to discuss only a typical case of \( z = 19 \). The expected emission of the same emission lines from different redshifts can also have the similar flux level. This realises because the flux per frequency has apparently positive effect of the redshift (e.g. Eq.(6) of Ciardi & Ferrara 2001) and the sound speed at the primordial starforming region should also be redshifted (Kamaya & Silk 2001). Furthermore, our estimate is reasonable if we do not consider smaller \( z \) than \( \sim 6 \) at which the reionisation of the Universe occurs and the adopted assumptions for analysis break.

In the current paper, we need the redshifted observational frequency and wavelength. For the three lines, we obtain \( 0.53 \times 10^{12} \) Hz; \( 5.6 \times 10^{-1} \) mm for \( J = 2 - 0 \) of \( \text{H}_2 \), \( 0.53 \times 10^{12} \) Hz; \( 5.6 \times 10^{-1} \) mm for \( J = 4 - 3 \) of HD, and \( 3.7 \times 10^{12} \) Hz; \( 8.1 \times 10^{-1} \) mm for \( J = 17 - 16 \) of LiH. The adopted \( 1+z \) is 20 according to the results of recent numerical simulations. Obviously, the predicted frequency is located in the range of ALMA. Hence, we discuss the observational possibility of detection by ALMA in the current paper. ALMA is a ground-based radio interferometric facility, and will consist of 96 12-m antennas. A detailed recent review is found in Takeuchi et al. (2001). According to this, the 5\( \sigma \) sensitivities at 350 \( \mu \)m, 450, 650, 850, 1.3 mm, 3.0 mm are expected to be 390, 220, 120, 16, 7.5, 4.6 \( \mu \)Jy, respectively (8-GHz bandwidth).

The most prominent feature is predicted to be a double peak of HD and \( \text{H}_2 \) emission. A schematic view is presented in figure 5, but it is depicted at the coordinate of the core (i.e. they are not redshifted). The most obvious feature is the difference of the peaks of each line intensity. The ratio of \( \text{H}_2 \) to HD is about 50. Detection of this double peak feature would confirms the presence of primordial molecules in forming galaxies. The difference in frequency of both the molecules is about \( 10^{8} \) Hz. Each of the precise values is \( 5.3317 \times 10^{11} \) Hz for \( \text{H}_2 \) \((J=2-0)\) and \( 5.53338 \times 10^{11} \) Hz for HD \((J=4-3)\), respectively. The frequency difference is resolved sufficiently by ALMA since it has frequency resolution of about \( 4 \times 10^4 \) Hz.

To estimate the observed flux, we determine the distance to the object. Then, we
calculate it numerically from the following standard formula:

\[ D_{19} = \frac{c}{H_0} \int_0^{19} \frac{dz}{(\Omega_\Lambda + \Omega_M(1+z)^3)^{0.5}} \]  

(14)

where \( H_0 \) is the Hubble parameter taken to be 75 km sec\(^{-1}\) Mpc\(^{-1}\), \( \Omega_\Lambda \) is the cosmological constant parameter, and \( \Omega_M \) is the density parameter. We consider the case \( \Omega_\Lambda + \Omega_M = 1 \), since our discussion bases on the numerical results (e.g. Abel et al. 2000). Adopting \( D_{19} \), we obtain the observed fluxes of each of the lines. The results are summarised in table 1.

Although the line-broadening is estimated from \( \nu_0 \delta v_D / c \), we also correct it for the redshift effect (\( \nu_0 \) is the central frequency). For each of the parameter sets of \( (\Omega_\Lambda, \Omega_M) \), we obtain \( D_{19} = 0.62 \times 10^{10} \) pc (\( \Omega_\Lambda = 0, \Omega_M = 1 \)), \( D_{19} = 1.00 \times 10^{10} \) pc (\( \Omega_\Lambda = 0.7, \Omega_M = 0.3 \)), and \( D_{19} = 4.58 \times 10^{10} \) pc (\( \Omega_\Lambda = 0.9, \Omega_M = 0.1 \)). According to Table 1, the rotational line fluxes of \( J = 2 - 0 \) (\( v=0 \)) for H\(_2\) are 0.16 \( \mu Jy \); 0.0042 \( \mu Jy \) for \( J = 4 - 3 \) (\( v=0 \)) for HD; and 0.0000041 \( \mu Jy \) for \( J = 17 - 16 \) (\( v=0 \)) for LiH if \( \Omega_M + \Omega_\Lambda = 1 \). Thus, we conclude that a single core is not easily observable even by ALMA.

However we note that if the cores are collectively assembled on a sub-galactic scale (Shchekinov 1991), the agglomeration can be detected by ALMA (Kamaya & Silk 2001). We shall estimate the number of cores in a primordial galaxy. Firstly, we must consider the lifetime of a core able to show double peak emission. The required density and temperature distribution for such a core is possible when the accretion rate of the contracting gas is about 0.01 \( M_\odot \) year\(^{-1}\) (Omukai & Nishi 1998; Kamaya & Silk 2001). Then, the life-time of the core with double peak emission is about \( 10^4 \) years as long as a massive star of \( \sim 100 M_\odot \) forms inside the core. A \( 10^6 M_\odot \) cloud (Abel et al. 2000) is expected to form 1000 such cores at a plausible efficiency of 0.01 in mass during its life-time. Taking its lifetime to be \( \sim 10^5 \) years as the free-fall time of a \( 10^6 M_\odot \) cloud, we find that its luminosity can reach \( 100 L_{\text{single}} \).

Next, we consider an entire primordial galaxy with \( 10^{11} M_\odot \). It may form \( 10^{7} \) supernovae over its entire lifetime. We assume that it makes \( 10^7 \) primordial massive stars, since this number of massive stars gives enrichment to roughly 1 percent of the solar metallicity. If the burst of formation of primordial molecular cloud cores occurs in the central region of the primordial galaxy (we postulate 1 kpc as the size of the core-forming region), then there are \( 10^4 \) such giant molecular clouds with \( 10^6 M_\odot \) in the core-forming region, as long as the massive star forms with a high accretion rate of 0.01 \( M_\odot \) year\(^{-1}\) (Kamaya & Silk 2001). During this phase, the cumulative luminosity would be \( 10^6 L_{\text{single}} \). However, the dynamical time-scale in the core-forming region may be \( \sim 10^7 \) years (e.g. the duration of the starburst). Then, we obtain \( 10^4 L_{\text{single}} \) for the luminosity of the primordial galaxy undergoing its first star formation burst, conservatively assuming \( \sim 10^5 \) years as the life-time of giant molecular clouds. Finally, for molecular-line emitting proto-galaxies, we obtain 1.6 mJy for \( J = 2 - 0 \).
of H$_2$, 0.43 mJy for $J = 4 - 3$ of HD and 0.00001 mJy for $J = 17 - 16$ of LiH ($\Omega_M = 0.3$ and $\Omega_\Lambda = 0.7$). The estimated flux levels of H$_2$ and HD are consistent with Shchekinov (1991), in which only the lowest transition lines for both the molecules were discussed. It may also be better to say that these values are optimistic values. In more realistic conditions, furthermore, our simple time-dependent summation scheme might break down.

According to the current status of the instrumentation for ALMA, 80-890 GHz is the allowed detectable range. It is feasible for our prediction of the redshifted emission. Unfortunately, however, the transmission is bad for the predicted feature at 530 GHz because of the atmosphere of the Earth. Then, it may be necessary to detect H$_2$ and HD emission from a protogalaxy forming larger than $1 + z = 20$. Since $\Omega_M < 1$, which seems to be reasonable if $\Omega_\Lambda = 0.7$, the formation of the cores is prompted. Then, we can expect to detect emission at a larger frequency than 530 GHz, and detection should be feasible of the H$_2$ and HD double emission from the assembly of the primordial molecular cores. Of course, we also expect the emission later than $1 + z = 20$, since the Universe has been reionised at $z \sim 6$. The latter case is also favourable for ALMA because of the better sensitivity.

In the previous paper, we advocated a deep blank field survey. Then, in the current paper, we propose another observational strategy to detect the double emission feature from the primordial molecular cloud cores. Measurement of the number counts of submillimeter sources is planned as one key galaxy evolution project for ALMA (Takeuchi et al. 2001). According to the predictions, many submillimeter sources are expected below sub-mJy levels. Once the survey is operating, we can utilise the submillimeter source count data. Firstly, we pick up the faint sources around QSOs since QSOs are expected at high density peaks in the usual hierarchical model of cosmic structure formation from primordial Gaussian-distributed density fluctuations. Primordial galaxies are concentrated around QSOs. Secondly, we roughly check the spectra. Primordial galaxies do not have dust, while evolved systems have dust. This means the continuum level of the flux at submillimeter wavelengths is significantly different between primordial and evolved galaxies. Unfortunately, it seems that the faint sources are observed in the low frequency resolution mode according to Takeuchi et al. (2001). But, one can expect to find unresolved double peaks as a bump in the observed spectral energy distribution, which is a different feature from the blackbody emission by dust. To find the bump due to the double emission lines should not be a difficult task. After this simple selection, we re-observe the candidates for primordial submillimeter sources in the high resolution mode in frequency. Finally, it is expected that the primordial cores can be discovered showing the double peak spectral features due to H$_2$ and HD, in which the ratio of the two peaks, which is about 50, confirms the hypothesis of primordial emission.

Finally, we stress that we are able to recognise the difference between H$_2$ emission
from the assembly of primordial molecular clouds and that supernova shells in primordial starforming regions (Ciardi & Ferrara 2001). According to figure 1 of Ciardi & Ferrara, the emission of the ground rotational line of H$_2$ ($v = 0$), which is never the dominant cooling line because of the high temperature of the shell, can have a flux level of sub-mJy to mJy at $z \sim 10$. This flux level is obtained via adoption of the sound velocity of 10 km sec$^{-1}$ in the shell gas. Thus, both our predictions and those of Ciardi & Ferrara yield similar flux levels for the same molecular line of H$_2$. The difference between the two predictions is the HD line to be associated with the H$_2$ line in our case. To conclude, if and when the double peak emission is found, it would strongly indicate the primordial emission from the assembly of the first starforming molecular clouds.

6. THEORY OF DOUBLE PEAK EMISSION

How is the double-peak emission produced? We describe a theory for double-peak emission from primordial molecular cloud cores. In the entire region of the core, the temperature is significantly lower than 515 K which corresponds to the transition energy of H$_2$ (J=2-0). Such low temperatures are possible only when HD cooling is efficient. Then, the effect of the large volume of the low temperature region lets the first and larger peak be a rotational emission line of H$_2$ (J=2-0). This is possible because of the thermalisation of the gas as long as the gas temperature is above 100 K (i.e. $\sim 2^2 \times 85 \times 2/7; \text{J}=2$), since the rotational level of $\text{J}=2$ is excited by chance.

The situation of the second peak is a little more complicated. We define a characteristic density for the three-body reaction to set in as being $n_{\text{three}} \sim 10^8$ cm$^{-3}$. Around the region of this density, the cooling rates of HD and H$_2$ are comparable. Once it is confirmed that the temperature is determined by the balance of the cooling of HD and H$_2$ with adiabatic heating, we find that a temperature of $\sim 300$ K at a density of $n_{\text{three}}$ is realized. In other words, if the cooling of H$_2$ were to be neglected, the temperature would be lower than 300 K since the corresponding heating was not allowed there. By the way, since the temperature of 300 K permits the thermal excitation of $J = 4$ of HD, then the rotational emission of HD (J=4-3) becomes possible. This emission occurs since the gas temperature can reach 300 K because of the H$_2$ cooling balancing the adiabatic heating of the gravitationally contracting core. This efficiency of H$_2$ cooling is realized only when the three-body reaction among H atoms occurs. Thus, the second peak is possible owing to the three-body reaction to form H$_2$. 
7. SUMMARY

One of the main goals of cosmology is to find the first generation of stars. When they form, strong H$_2$ emission and weak HD emission is expected as a double peak feature. The weak HD emission is important since it distinguishes between the H$_2$ emission from the primordial molecular clouds and that from the primordial supernova shell (Ciardi & Ferrara 2001). We have examined the observational feasibility of the detection of the double peak emission. According to our analysis, the double peak feature is marginally detectable by ALMA. However, the transmissivity of air for the expected typical emission is low for the ALMA project as pointed out in our previous paper. If future telescopes are able to detect the double peak feature emission from primordial molecular cloud cores, then either primordial cores and the first stars have formed at different redshift from $z = 19$.

H.K. is grateful to Profs. S.Inagaki, S.Mineshige, and Yu.Shchekinov for their encouragement.
APPENDIX

We re-formulate the energy loss due to line emission of H$_2$. The details are found in Kamaya & Silk (2001). Line emission of H$_2$ occurs due to the changes among rotation and vibration states. We can basically use the formulation of Hollenbach & McKee (1979) for rotational and vibrational emission of H$_2$. Adopting their notation, we get:

\[
L_r \equiv \left( \frac{9.5 \times 10^{-22} T_3^{3.76}}{1 + 0.12 T_3^{2.1}} \exp \left[ - \left( \frac{0.13}{T_3} \right)^3 \right] \right) + 3.0 \times 10^{-24} \exp \left( - \frac{0.51}{T_3} \right) \text{ erg s}^{-1}, \tag{A1}
\]

then, we estimate the cooling rate as

\[
\Lambda(\text{rot}) = n_{\text{H}_2} L_r (1 + \zeta_{\text{H}_2})^{-1} + n_{\text{H}_2} L_r (1 + \zeta_{\text{H}_2 r})^{-1} \text{ erg cm}^{-3} \text{ s}^{-1}, \tag{A2}
\]

where \( \zeta_{\text{H}_2} = n_{\text{H}_2\text{cd}}(\text{rot})/n_{\text{H}} \), \( \zeta_{\text{H}_2 r} = n_{\text{H}_2\text{cd}}(\text{rot})/n_{\text{H}_2} \), \( n_{\text{H}_2\text{cd}}(\text{rot}) = A_J/\gamma_{J}^{\text{H}_2} \), and \( A_J \) is the Einstein A value for the \( J \) to \( J - 2 \) transition; \( \gamma_{J}^{\text{H}_2} \) is the collisional de-excitation rate coefficient due to neutral hydrogen; and \( \gamma_{J}^{\text{H}_2} \) is that due to molecular hydrogen. The first term of \( L_r \) denotes the cooling coefficient due to the higher rotation level (\( J > 2 \)) and the second one due to \( J = 2 \rightarrow 0 \) transition. The vibrational levels of both terms are set to be zero.

For the vibrational transitions,

\[
L_v = 6.7 \times 10^{-19} \exp \left[ - \left( \frac{5.86}{T_3} \right)^3 \right] + 1.6 \times 10^{-18} \exp \left( - \frac{11.7}{T_3} \right) \text{ erg s}^{-1}, \tag{A3}
\]

then, we get the cooling rate as being

\[
\Lambda(\text{vib}) = n_{\text{H}_2} L_v (1 + \zeta_{\text{H}_v})^{-1} + n_{\text{H}_2} L_v (1 + \zeta_{\text{H}_2 v})^{-1} \text{ erg cm}^{-3} \text{ s}^{-1}, \tag{A4}
\]

where \( \zeta_{\text{H}_v} = n_{\text{H}_2\text{cd}}(\text{vib})/n_{\text{H}} \), and \( \zeta_{\text{H}_2 v} = n_{\text{H}_2\text{cd}}(\text{vib})/n_{\text{H}_2} \). Here, \( n_{\text{H}_2\text{cd}}(\text{vib}) = A_{ij}/\gamma_{ij}^{\text{H}_2} \) and \( n_{\text{H}_2\text{cd}}(\text{vib}) = A_{ij}/\gamma_{ij}^{\text{H}_2} \) where \( A_{ij} \) is the Einstein A value for the \( i \) to \( j \) transition; \( \gamma_{ij}^{\text{H}_2} \) is the collisional de-excitation rate coefficient due to neutral hydrogen; and \( \gamma_{ij}^{\text{H}_2} \) is that due to molecular hydrogen. In our formula, only the levels of \( v = 0, 1 \) and \( 2 \) are considered. This is sufficient since the temperature is lower than 2000 K. The first term of \( L_v \) is a cooling coefficient of \( \delta v = 1 \) and the second term is that of \( \delta v = 2 \). The second term has effect on only the central region of our structural model, then it has no significant contribution to our conclusion. Combining Eq.(A2) and Eq.(A4), we obtain the total cooling rate as \( \Lambda^{\text{thin}} = \Lambda(\text{rot}) + \Lambda(\text{vib}) \) erg cm$^{-3}$ s$^{-1}$ in the optically thin regime. When we need a cooling function which can be used in the optically thick regime, \( \Lambda^{\text{thin}} \) is multiplied by the escape probability like the other cooling function in the main text.
It may be better to comment on the continuum absorption. The effect of the continuum absorption below 2000 K would be multiplied by \( \exp(-\tau_{cont}) \), in which

\[
\tau_{cont} = \rho(r)\lambda_J \left[ 4.1 \left( \frac{1}{\rho(r)} - \frac{1}{\rho_0} \right)^{-0.9} T_3^{-4.5} + 0.012\rho^{0.51}(r)T_3^{2.5} \right]
\]

(A5)

according to the estimate of Lenzuni, Chernoff, & Salpeter (1991) who obtain a fitting formula for the Rossland mean opacity in a zero-metallicity gas. Here, \( \lambda_J \) is the Jeans length and \( \rho_0 \) is 0.8 g cm\(^{-3} \). Their fitting formula is reasonable if we consider the temperature range \( T > 1000 \) K. Our lowest temperature of the collapsing core is about 50 K. Then, their formula may not be appropriate, while it gives an sufficiently upper limit if we adopt \( \tau_{cont} \) of 1000 K instead of really having \( \tau_{cont} \) below 1000 K. For all of our estimates, \( \tau_{cont} \) is much smaller than unity. Then, we can neglect the effect of continuum absorption.

We summarise the parameters in our calculation for a rotational transition with \( v = 0 \); \( A_{2,0} = 2.94 \times 10^{-11} \) sec\(^{-1} \); and \( A_{J,J-2} = 5A_{2,0}/162 \times J(J-1)(2J-1)^4/(2j+1) \) sec\(^{-1} \) are considered. For a vibrational transition, \( A_{10} = 8.3 \times 10^{-7} \) sec\(^{-1} \); \( A_{21} = 1.1 \times 10^{-6} \) sec\(^{-1} \); and \( A_{20} = 4.1 \times 10^{-7} \) sec\(^{-1} \) are considered. In the main text, we find that the rotational line cooling of H\(_2\) is dominated by \( J = 2 - 0 \) transition (\( v = 0 \)). Then, we regard that the second term of Eq.(A1) is important. This means our estimate for \( J = 2 - 0 \) transition is very reliable, while the other estimate has some uncertainty.

Finally, we comment on the uncertainty of the cooling function owing to rot-vibrational transitions of H\(_2\). The formula for the cooling function of H\(_2\) is examined by Martin et al. (1996), Forrey et al. (1997), Galli & Palla (1998), and Fuller & Couchman (2000). Fuller & Couchman especially stress that there is uncertainty in the H\(_2\) cooling function because of the difficulty in calculating the interaction potential at low temperatures. Then, different choices for rotational and vibrational H-H\(_2\) rate coefficients will produce differences in the cooling function. Fortunately, we can consider our cooling function to be applicable since the cooling rate via H\(_2\) transitions balances the release of gravitational potential energy consistently as shown in our first paper (Kamaya & Silk 2001).
REFERENCES

[29] Shchekinov Yu., 1986, SvAL, 12, 211
Table 1: Expected Emission Lines

<table>
<thead>
<tr>
<th></th>
<th>$H_2$ ($J = 2 - 0$)</th>
<th>HD ($J = 4 - 3$)</th>
<th>LiH ($J = 17 - 16$)</th>
<th>$\Omega_m$</th>
<th>$\Omega_\Lambda$</th>
<th>$D_{19}$ ($10^{10}$ pc)</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\nu$ ($10^{13}$ Hz; $z = 0$)</td>
<td>1.06</td>
<td>1.06</td>
<td>0.74</td>
<td>–</td>
<td>–</td>
<td>–</td>
</tr>
<tr>
<td>$\nu$ ($10^{12}$ Hz; $z = 19$)</td>
<td>0.53</td>
<td>0.53</td>
<td>0.37</td>
<td>–</td>
<td>–</td>
<td>–</td>
</tr>
<tr>
<td>$\lambda$ ($10^{-3}$ mm; $z = 0$)</td>
<td>28.29</td>
<td>28.29</td>
<td>40.30</td>
<td>–</td>
<td>–</td>
<td>–</td>
</tr>
<tr>
<td>$\lambda$ ($10^{-3}$ mm; $z = 19$)</td>
<td>565.8</td>
<td>565.8</td>
<td>806.1</td>
<td>–</td>
<td>–</td>
<td>–</td>
</tr>
<tr>
<td>$L_\nu$ ($10^{26}$ erg sec$^{-1}$ Hz$^{-1}$)</td>
<td>40.1</td>
<td>1.03</td>
<td>0.001</td>
<td>–</td>
<td>–</td>
<td>–</td>
</tr>
<tr>
<td>$f_\nu$ ($10^{-8}$ Jy; $z = 19$)</td>
<td>43.18</td>
<td>1.09</td>
<td>0.0003</td>
<td>1.0</td>
<td>0.0</td>
<td>0.62</td>
</tr>
<tr>
<td>$f_\nu$ ($10^{-8}$ Jy; $z = 19$)</td>
<td>16.60</td>
<td>0.42</td>
<td>0.0001</td>
<td>0.3</td>
<td>0.7</td>
<td>1.00</td>
</tr>
<tr>
<td>$f_\nu$ ($10^{-8}$ Jy; $z = 19$)</td>
<td>7.58</td>
<td>0.19</td>
<td>0.00004</td>
<td>0.1</td>
<td>0.9</td>
<td>1.48</td>
</tr>
</tbody>
</table>
Fig. 1.— Density–H$_2$ fraction relation (solid line) and Density–Temperature relation (dashed line) are depicted. Using Eq.(8), we translate them to Radius–Density and –Temperature relations, respectively.
Fig. 2. — Cooling rate: HD (solid), H$_2$ (short dashed), LiH (long dashed), and total (dotted).

Below $\sim 10^8$ cm$^{-3}$, HD is dominant, while H$_2$ is important above the density. LiH is not so significant because of the lines of LiH are optically thick.
Fig. 3.— Heating rate: compressional (solid), reactive (dashed), and total (dotted).
Fig. 4 — Ratio of cooling to heating. As found deeply, our model is reasonable almost a few factors. This supports our model structure of a molecular cloud core.
Fig. 5.— Schematic view of the double peak emission of H$_2$ and HD. The difference between the two lines is about $5.0 \times 10^{10}$ Hz. This is resolved by ALMA project.