Mon. Not. R. Astron. Soc. **361,** 850–854 (2005) doi:10.1111/j.1365-2966.2005.09226.x

The cooling function of HD molecule revisited

Anton Lipovka,[1⋆] Ramona Núñez-López[1,2] and Vladimir Avila-Reese[2]

[1]*Centro de Investigación en Física, UNISON, Rosales y Blvd. Transversal, Col. Centro, Edif. 3-I, Hermosillo, Sonora, 83000, México*
[2]*Instituto de Astronomía, U.N.A.M., A.P. 70-264, 04510, México, D.F., México*

Accepted 2005 May 20. Received 2005 May 10; in original form 2005 March 30

ABSTRACT

We report new calculations of the cooling rate of primordial gas by the HD molecule, taking into account its ro-vibrational structure. The HD cooling function is calculated including radiative and collisional transitions for $J \leqslant 8$ rotational levels, and for the vibrational levels $v = 0$, 1, 2 and 3. The ro-vibrational level population is calculated from the balance equation assuming steady state. The cooling function is evaluated in the ranges of the kinetic temperatures, $T_{\rm k}$, from 10^2 to 2×10^4 K and the number densities, $n_{\rm H}$, from 1 to 10^8 cm^{-3}. We find that the inclusion of collisional ro-vibrational transitions increases significantly the HD cooling efficiency, in particular for high densities and temperatures. For $n_{\rm H} \gtrsim 10^5$ and $T_{\rm k} \sim 10^4$ K the cooling function becomes more than an order of magnitude higher than previously reported. We give also the HD cooling rate in the presence of the cosmic microwave radiation field for radiation temperatures of 30, 85 and 276 K (redshifts of 10, 30 and 100). The tabulated cooling functions are available at http://www.cifus.uson.mx/Personal_Pages/anton/DATA/HD_cooling/HD_cool.html. We discuss the relevance to explore the effects of including our results into models and simulations of galaxy formation, especially in the regime when gas cools down from temperatures above ∼3000 K.

Key words: molecular processes – galaxies: formation – cosmology: miscellaneous.

1 INTRODUCTION

The cooling and thermal balance of the primordial, zero-metallicity gas by molecular hydrogen (H_2) and deuterated hydrogen (HD) are key ingredients in the formation process of the first baryonic objects in the universe, such as dwarf-sized galaxies and Pop-III stars (see for recent reviews on this topic Barkana & Loeb 2001; Bromm & Larson 2004; Ciardi & Ferrara 2005). It is well known that H_2 and HD molecules form in the universe after recombination (e.g. Lepp & Shull 1984; Puy et al. 1993; Palla, Galli & Silk 1995; Galli & Palla 1998; Stancil, Lepp & Dalgarno 1998). The formation of H_2 and HD molecules in primordial gas is also possible in a post-shock flow (Mac Low & Shull 1986; Shapiro & Kang 1987; Uehara & Inutsuka 2000), where the gas density and temperature, as well as the molecular fractions, are different from those of the expanding homogeneous gas.

The H_2 molecule is considered typically as the main coolant in the primordial medium (e.g. Tegmark et al. 1997; Abel, Bryan & Norman 2000; Bromm, Coppi & Larson 2002). Thus, rather detailed calculations were carried out for it (see for the most recent results Le Bourlot, Pineau des Forêts & Flower 1999; Flower et al. 2000; Shaw et al. 2005, and references therein). Nevertheless, in the case of dense primordial gas, the role of the HD molecule in the thermal and cooling process may become comparable to or more important than the one of H_2. Therefore, detailed calculations of the HD cooling function (the rate of cooling per HD molecule, hereafter CF) are needed.

The HD molecule is an efficient coolant in the primordial medium because it has a permanent electric dipole moment that allows high probabilities for the radiative rotational transitions from the rotational levels pumped by collisions with H and He. Besides the HD molecule was efficiently produced in the reaction of chemical fractionation $D^+ + H_2 \rightarrow H^+ + HD$, which leads to a strong enhancement of the initial abundance of HD, up to roughly $[HD]/[H_2] = 10^{-2}$ to 10^{-3} (e.g. Puy et al. 1993; Galli & Palla 1998; Flower 2000). The HD molecule can cool the primordial gas to temperatures below ∼300 K because it allows dipole rotational transitions characterized by energies two times smaller than those of the quadrupole transitions of H_2. Regarding higher temperatures ($\gtrsim 3000$ K), cooling by HD can be again as important as that by H_2. This question will be discussed in the present paper.

The HD CF was calculated for the first time by Dalgarno & McCray (1972) for low temperatures and Boltzmann-distributed rotational level populations. Varshalovich & Khersonskii (1976) improved the calculations by taking into account the departure from local thermodynamic equilibrium. More recently, Flower (2000; also see references therein) have calculated the HD CF for low and intermediate kinetic temperatures and a large range of densities. These authors considered the rotational transitions within the

⋆E-mail: aal@cajeme.cifus.uson.mx

vibrational ground state ($v = 0$) of HD. Note that in the case of higher kinetic temperatures ($T_k \gtrsim 2 \times 10^3$ K), the populations of the vibrational levels become significant, and cooling by ro-vibrational transitions of HD may be important due to (i) the relatively high energy of vibrational quanta, and (ii) the relatively high probabilities of the ro-vibrational radiative transitions. Therefore, the inclusion of the vibrational structure of the HD molecule in the calculation of its CF might be important.

The aim of this paper is to recalculate the HD CF for a wide range of kinetic temperatures and densities by taking into account ro-vibrational transitions within ground ($v = 0$) and the first three excited ($v = 1, 2, 3$) vibrational levels. Further exploration of the influence of the HD CF calculated here on the thermal evolution of the primordial medium will be presented elsewhere. In Section 2, we give details of our calculations. The revised HD CF is given and compared with that from Flower et al. (2000) in Section 3. Finally, in Section 4 we discuss our results and speculate about possible implications.

2 THE MODEL

It is well known that in the low-density limit ($n_H < 10^3$ cm^{-3}), the relative populations of the levels of HD molecule depart significantly from the Boltzmann distribution. Therefore, to calculate the HD CF in the general case, we need the correct values of the ro-vibrational level populations outside the thermodynamical equilibrium. This can be calculated by using the equations of detailed population level balance

$$n_{vJ} \sum_{v'J'} \left(W^{R}_{vJ\rightarrow v'J'} + W^{C}_{vJ\rightarrow v'J'} \right) = \sum_{v'J'} n_{v'J'} \left(W^{R}_{v'J'\rightarrow vJ} + W^{C}_{v'J'\rightarrow vJ} \right); \qquad \sum_{vJ} n_{vJ} = 1, \tag{1}$$

where n_{vJ} is the population of the ro-vibrational level vJ, $W^{R}_{vJ\rightarrow v'J'}$ and $W^{C}_{vJ\rightarrow v'J'}$ are the probabilities of the radiative and collisional transitions, respectively. We assume a steady state for the population levels. This assumption has been used and discussed to be valid in our context by many other authors (e.g. Flower et al. 2000; Flower & Pineau des Forêts 2001; Le Petit, Roueff & Le Bourlot 2002).

The population of the ro-vibrational levels of the *HD* molecule was calculated in the wide range of number densities n_H from 1 to 10^8 cm^{-3}, and for the kinetic temperature T_k from 10^2 to 2×10^4 K. The ro-vibrational radiative transition probabilities for the HD molecule were taken from Abgrall, Roueff & Viala (1982). Regarding the collisional transition probabilities, it was shown in Flower et al. (2000) that the HD CF is insensitive to the H/H_2 density ratio. Therefore, one may take into account the excitation and de-excitation of HD only by collisions with the H atoms. The probabilities of the collisionally excited pure rotational transitions of HD (up to the third vibratioanally excited state, $0 \leqslant v \leqslant 4$, and up to the 8th rotational level $0 \leqslant J \leqslant 8$) were taken from Roueff & Flower (1999) and Roueff & Zeippen (1999). We consider only the dipolar transitions ($\Delta J = \pm 1$). Owing to the permanent dipolar moment of the HD molecule, these transitions dominate collisional population transfer (Flower & Roueff 1999). Flower & Roueff (1999) computed probability coefficients for several ro-vibrational transitions in HD induced by collisions with atomic and molecular hydrogen in a range of temperatures from 100 to 2000 K. In that paper, some values of the transition probabilities for the vibrational relaxation $v = 1 \rightarrow 0$ are presented and compared with the corresponding coefficients for H_2. The rate coefficients for vibrational relaxation of HD and H_2 in collisions with H are similar in magnitude for a given temperature. Besides, the probabilities for both molecules change approximately in the same way with temperature. On the basis of these results and in the absence of extensive calculations for the HD+H collisional ro-vibrational transition probabilities in the range of temperatures we want to explore, we will use the corresponding probabilities of the H_2+H (Tiné, Lepp & Dalgarno 1998) given in electronic form on the website http://www.physics.unlv.edu/astrophysics/h2h2rates/index.html.

The total CF per unit of volume is defined, for example, for the HD molecule, as

$$\Lambda_{HD} = n_{HD} W_{HD}, \tag{2}$$

where n_{HD} is the HD number density, and W_{HD} is the HD CF in units of erg s^{-1} per HD molecule

$$W_{HD} = \sum_{vJv'J'} \left(n_{vJ} W^{R\downarrow}_{vJ\rightarrow v'J'} - n_{v'J'} W^{R\uparrow}_{v'J'\rightarrow vJ} \right) h\nu_{vJ\rightarrow v'J'}. \tag{3}$$

Here, $W^{R\downarrow}_{vJ\rightarrow v'J'} = A^{R\downarrow} + B^{R\downarrow}\mathbf{u}$ are the probabilities of the radiative transitions with the emission of the photon $h\nu_{vJ\rightarrow v'J'}$, and $W^{R\uparrow}_{v'J'\rightarrow vJ} = B^{R\uparrow}\mathbf{u}$ are the probabilities of radiative transition with the absorption of the corresponding field photon. The symbols A and B are for the corresponding Einstein coefficients and $\mathbf{u}$ is the radiation field. The populations of the ro-vibrational levels n_{vJ} are those calculated from the balance equation (1). This definition of W_{HD} is more general than the one used in Flower et al. (2000), because it takes into account the potential effects of a radiation field in the cooling process. In the case of $T_r << T_k$, equation (3) tends to the case considered in Flower et al. (2000). At high redshifts, the cosmic microwave background radiation (CMBR) temperature, $T_r = T_{CMBR}$, may become comparable to the kinetic temperature of the gas T_k; this will significantly affect the HD CF at that T_k (see below for more details).

3 THE COOLING FUNCTION OF HD MOLECULE

In Fig. 1 we present the variation of W_{HD} with T_k and n_H. The dotted-line curves correspond to the HD CF, neglecting the collisional ro-vibrational transitions as in Flower et al. (2000). Our results agree well with those of these authors. Note that we did not consider collisions of HD with He and H_2 because, as it was mentioned above, Flower et al. (2000) showed that W_{HD} is essentially a function of T_k and n_H only. The solid-line curves in Fig. 1 are the CFs including ro-vibrational collisional transitions for a four-level vibrational structure of the HD molecule ($v = 0, 1, 2, 3$). One sees that the latter CFs depart from the former, as T_k and n_H are larger. For $n_H \gtrsim 10^6$ cm^{-3} and $T_k \approx 10^4$ K, the calculated value of W_{HD} including the vibrational transitions is more than a factor of 50 larger than the W_{HD} calculated neglecting collisional ro-vibrational transitions. Note that in Fig. 1, W_{HD} has been calculated for $T_r = 2.73$ K (the CMBR temperature at present), i.e. well within the limit $T_r << T_k$, when the radiation field does not participate in the thermal balance of the gas and equation (3) is reduced to the equation for W_{HD} used in Flower et al. (2000). This way we are able to compare our results with those of these authors.

The exact HD CF data presented here are available at http://www.cifus.uson.mx/Personal_Pages/anton/DATA/HD_cooling/HD_cool.html. To facilitate the use of the HD CF in computational programs we give also a polynomial approximation

Table 1. Polynomial coefficients D_{lm}.

	$m=0$	$m=1$	$m=2$	$m=3$	$m=4$
$l=0$	−42.576 88	0.924 33	0.549 62	−0.076 76	0.002 75
$l=1$	21.933 85	0.779 52	−1.064 47	0.118 64	−0.003 66
$l=2$	−10.190 97	−0.542 63	0.623 43	−0.073 66	0.002 514
$l=3$	2.199 06	0.117 11	−0.137 68	0.017 59	−0.000 666 317
$l=4$	−0.173 34	−0.008 35	0.0106	−0.001 482	0.000 061 926

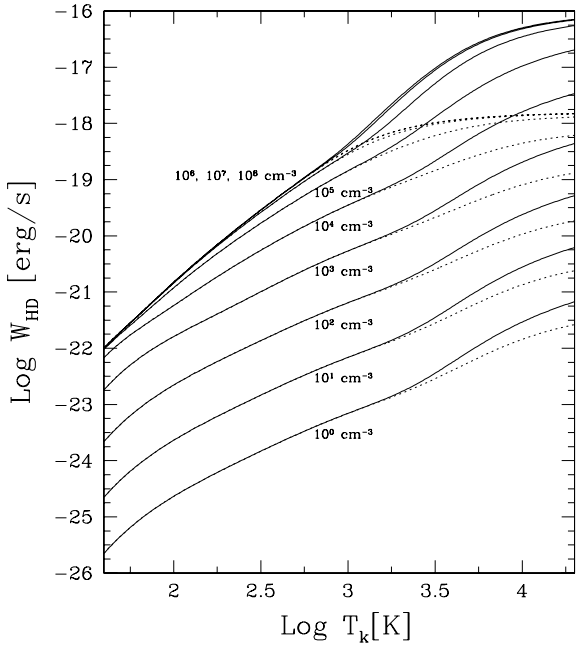

Figure 1. Cooling function of the HD molecule, calculated from $n_{\rm H}$ = 1–10^8 cm^{-3} in powers of 10 (from bottom to top). Radiation temperature, $T_{\rm r}$, was set equal to 2.73 K ($T_{\rm r} \ll T_{\rm k}$). Solid curves correspond to the cases when collisional ro-vibrational transitions ($v = 0$, 1, 2, 3, and $J \leqslant 8$) were taken into account, while dotted curves are for the case when these transitions were neglected in the calculations. The latter curves can be compared with those of fig. 3 in Flower et al. (2000). Note that the curves in both cases saturate for $n_{\rm H} \gtrsim 10^5$–10^6.

for the HD CF. The approximation is very accurate in the ranges of $n_{\rm H}$ and $T_{\rm k}$ studied here, from 1 to 10^8 cm^{-3}, and from 10^2 to 2×10^4 K, respectively. The approximation is writen in the form

$$\mathrm{Log}(W_{\rm HD}) = \sum_{l,m=0} D_{lm} T_{\rm k}^{l} n_{\rm HD}^{m}, \tag{4}$$

where the coefficients D_{lm} are tabulated in Table 1.

From Fig. 1 one clearly sees how $W_{\rm HD}$ increases at high densities after including the collisional ro-vibrational level transitions. In the case of low densities, the contribution of these transitions to the cooling of HD is less important. Nevertheless, at high temperatures $W_{\rm HD}$ is still larger than in the case when these transitions are omitted (pure rotational transitions shown by dashed line in Fig. 1). Therefore, the analytical approximation commonly used for the low-density limit (see e.g. Galli & Palla 2002) should be slightly modified. The approximation given in Galli & Palla (2002) is based on the calculations for only two low-rotational transitions $(J'J) = (10)$ and $(J'J) = (21)$, because the collisional probabilities of these transitions are rather large as compared to those of higher rotational levels. However, it should be stressed that when the vibrational structure is taken into account, then there are other ro-vibrational transitions with comparable probabilities of collisional excitation. Based on our results, we suggest the following modified approximation for the low-density limit HD CF:

$$\mathrm{Log}(W_{\rm HD}) = -42.459\,06 + 21.900\,83 T_{\rm k} - 10.1954 T_{\rm k}^2 + 2.197\,88 T_{\rm k}^3 - 0.172\,86 T_{\rm k}^4. \tag{5}$$

This approximation can be applied for the gas density $n_{\rm H}$ up to $10^3 - 10^4$ cm^{-3}.

The effects of the radiation field $\mathbf{u}$ in $W_{\rm HD}$ become important when $T_{\rm r} \approx T_{\rm k}$ (Flower 2000; Flower & Pineau des Forêts 2001). In this case, the radiative absorption by the HD molecule dominates, and the second term in equation (3), as well as the $B^{\rm R\downarrow}\mathbf{u}$ term in the probability $W^{\rm R\downarrow}_{vJ\to v'J'}$, should be considered. The second term in equation (2) can be interpreted as a heating function. At the redshfits at which the first baryon objects are expected to form ($z \approx$ 10–100), the CMB temperature can be similar to the typical kinetic temperatures of the small primordial gas clouds. In Fig. 2 we present the complete HD CFs (with the collisional ro-vibrational transitions included) considering a radiative field with $T_{\rm r} = T_{\rm CMBR}\,(0)(1+z)$ for redshifts z = 10, 30 and 100 (dotted, dashed and long-dashed lines, respectively) and for two densities, $n_{\rm H} = 10$ and 10^8 cm^{-3}. One sees that when $T_{\rm r} \approx T_{\rm k}$, $W_{\rm HD}$ falls dramatically. The second term in equation (3) actually comes to dominate and the HD molecular lines act as heating sources. This will inhibit the collapse of a gas cloud. Therefore the minimum temperature of the primordial collapsing clouds is limited by the CMBR temperature (or by the heating due to other radiation fields) and not by HD (and H_2) cooling.

We note that the steady-state assumption for the HD population levels (see Section 2) remains even at the high redshifts considered here. The typical time-scales for population level changes are determined mainly by the inverse of the transition Einstein coefficients. For the HD molecule transitions, these coefficients imply typical time-scales much less than the time-scales related to variations in $T_{\rm CMBR}$ and/or to the gas clouds' collapse in the epochs considered here ($z \lesssim 100$).

4 DISCUSSION

We have calculated the HD CF, $W_{\rm HD}$, for a wide range of kinetic temperatures and gas densities by taking into account the ro-vibrational structure of the molecule for both the radiative and collisional transitions. We have found that, including the collisional ro-vibrational transitions, the cooling efficiency of HD molecule is higher than previously reported. The main increase of $W_{\rm HD}$ as compared to previous works is at the high-temperature side and for high densities (see Fig. 1); for $n_{\rm H} > 10^5$ cm^{-3}, the differences in $W_{\rm HD}$ reach an order of magnitude and more at $T_{\rm k} \sim 10^4$. Our results, in support of recent claims (Flower 2000; Uehara & Inutsuka 2000; Flower & Pineau des Forêts 2001; Nakamura & Umemura 2002; Galli & Palla 2002), suggest that the HD molecule may play an important role in the thermal balance and cooling of primordial gas at high densities.

In Fig. 3 we attempt to compare the relative contributions to the CF of the gas by the H_2 and HD molecules. Because the ratio of abundances of HD to H_2 is significantly smaller than 1, the $W_{\rm HD}$ curves should be reduced by a factor equal to this ratio in order to compare the contributions to the cooling of gas by both molecules. As it was mentioned above, this ratio for the primordial gas, after chemical fractionation, is approximately 10^{-2} to 10^{-3}. In Fig. 3, we reduce $W_{\rm HD}$ by a factor of $[\mathrm{HD}]/[\mathrm{H_2}] = 10^{-2.4}$ according to Galli & Palla (2002) for $z = 10$. As one can see in Fig. 3, the role of HD

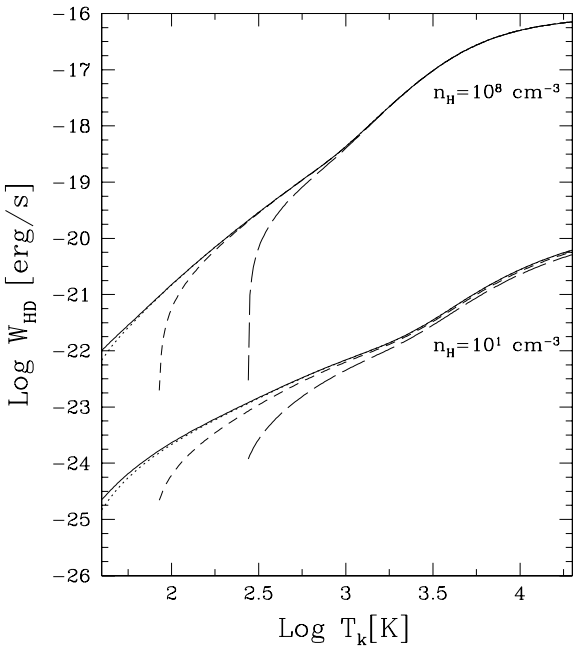

Figure 2. Cooling function of the HD molecule (including collisional rovibrational transitions) calculated for different values of the radiation temperature, $T_{\rm r} = 2.73(1+z)$ K, $z = 0$, 10, 30 and 100 (solid, dotted, dashed and long-dashed lines, respectively), and for $n_{\rm H} = 10$ and 10^8 cm^{-3}.

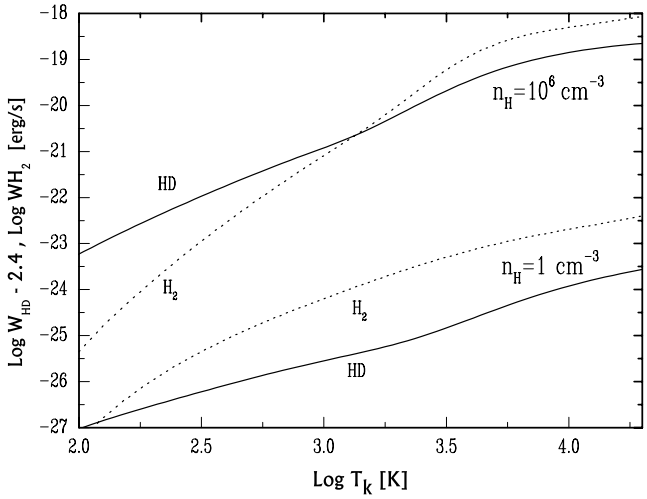

Figure 3. Cooling functions of the HD (solid lines) and H_2 (dashed lines) molecules for two gas densities, $n_{\rm H} = 1$ and 10^6 cm^{-3}, as indicated in the panel. To be compared, the HD CF was reduced by the factor $[{\rm HD}]/[{\rm H_2}] = 10^{-2.4}$. The H_2 CF is from Flower et al. (2000).

in the cooling of low-density gas is still unimportant with respect to the one of H_2, while for high densities, HD becomes as efficient a coolant as H_2, being even more efficient at low temperatures. The H_2 CF has been calculated according to Flower et al. (2000).

The contribution to the gas cooling of HD found here for high gas densities and temperatures larger than ∼3000 K is close to the corresponding contribution of H_2. This will surely affect calculations of galaxy formation in the regime when dense gas cools down from temperatures above ∼3000 K. This regime may arise in photoionization-heated gas or in shock-heated dense material in dwarf galaxy-size dark matter haloes with masses $\gtrsim 10^8$ $M_\odot$ (Bromm & Larson 2004). The presence of an efficient coolant, besides H_2, able to operate at $T_{\rm k} \sim 10\,000$ K and at high densities (as is the case of HD) is probably also relevant to understand the formation of the first globular clusters. Bromm & Clarke (2002) have shown that, under the action of an efficient coolant at $T_{\rm k} \lesssim 10\,000$ K, stellar clusters with masses $\sim 10^5$–10^7 may form into small dark matter subhaloes that later on are tidally destroyed during the violent relaxation of dwarf galaxy-sized haloes at $z \gtrsim 10$ (see also Weil & Pudritz 2001).

The cooling efficiency of H_2 or HD molecules increases with density until the population levels reach the local thermodynamical equilibrium at a critical density $n_{\rm c}$, in such a way that at $n_{\rm c}$ the probability of collisional de-excitation becomes equal to the spontaneous radiative probability. Beyond this density, the cooling is saturated. For molecular hydrogen, the critical density is rather low, $n_{\rm c,H_2} \sim 10^3$–10^4 cm^{-3}, due to the relatively small values of the H_2 Einstein coefficients. In the case of the HD molecule, the Einstein coefficients are larger as compared to those of H_2 by 2–3 orders of magnitude. One may estimate the ratio of critical densities $n_{\rm c,HD}/n_{\rm c,H_2}$ as $\approx A_{v'J'vj}({\rm HD})/A_{v'J'vj}({\rm H_2})$, which is $\approx 10^2$ for radiative vibrational transitions. The value of $n_{\rm c,HD}$ is indeed around 2 orders of magnitude higher than $n_{\rm c,H_2}$. From Fig. 1 (see also Flower et al. 2000), one sees that $n_{\rm c,HD} \approx 10^5$–$10^6$ cm^{-3}.

To conclude, we remark the importance of taking into consideration the HD CF calculated here in the simulations and models of the first baryonic objects in the universe. In particular, processes related to dense gas that cools down from temperatures above ∼3000 K will be affected by our results.

ACKNOWLEDGMENTS

This work was supported by grant PROMEP/103.5/03/1147 to AL. In addition, RNL gratefully acknowledges a PhD fellowship by CONACyT. We are grateful to J. Benda for grammar corrections to the manuscript, and C. Guzmán for computer assistance.

REFERENCES

Abel T., Bryan G., Norman M. L., 2000, ApJ, 540, 39
Abgrall H., Roueff E., Viala Y., 1982, A&ASS, 50, 505
Barkana R., Loeb A., 2001. Phys. Rep., 349, 125
Bromm V., Clarke C. J., 2002, ApJ, 566, L1
Bromm V., Larson R. L., 2004, ARA&A, 42, 79
Bromm V., Coppi P. S., Larson R. B., 2002, ApJ, 564, 23
Ciardi B., Ferrara A., 2005, Space Sci. Rev., 116, 625
Dalgarno A., McCray R. A., 1972, AR&A, 10, 375
Dalgarno A., Roberge W. G., 1979, ApJ, 233, L25
Flower D. R., 2000, MNRAS, 318, 875
Flower D. R., Pineau des Forêts G., 2001, MNRAS, 323, 672
Flower D. R., Roueff E., 1999, MNRAS, 309, 833
Flower D. R., Le Bourlot J., Pineau des Forets G., Roueff E., 2000, MNRAS, 314, 753
Galli D., Palla F., 1998, A&A, 335, 403
Galli D., Palla F., 2002, Planet. Space Sci., 50, 1197
Le Bourlot J., Pineau des Forêts G., Flower D. R., 1999, MNRAS, 305, 802
Le Petit F., Roueff E., Le Bourlot J., 2002, A&A, 390, 369
Lepp S., Shull J. M., 1984, ApJ, 280, 465
Nakamura F., Umemura M., 2002, ApJ, 569, 549
Mac Low M. M., Shull J. M., 1986, ApJ, 302, 89
Palla F., Galli D., Silk J., 1995, ApJ, 451, 44
Puy D., Alecian G., Le Bourlot J., Leorat J., Pineau Des Forets G., 1993, A&A, 267, 337
Roueff E., Flower D. R., 1999, MNRAS, 305, 353
Roueff E., Zeippen C. J., 1999, A&A, 343, 1005

Shapiro P. R., Kang H., 1987, ApJ, 318, 65
Shaw G., Ferland G. J., Abel N. P., Stancil P. C., van Hoof P. A. M., 2005, ApJ, 624, 794
Stancil P. C., Lepp S., Dalgarno A., 1998, ApJ, 509, 1
Tegmark M., Silk J., Rees M. J., Blanchard A., Abel T., Palla F., 1997, ApJ, 474, 1
Tiné S., Lepp S., Dalgarno A., 1998, Mem. Soc. Astron. Ital., 69, 345
Uehara H., Inutsuka S., 2000, ApJ, 531, L91
Varshalovich D. A., Khersonskii V. K., 1976, Sov. Astron. Lett., 2, 227
Weil M. L., Pudritz R. E., 2001, ApJ, 556, 164

This paper has been typeset from a TEX/LATEX file prepared by the author.