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Temperature and density dependent cooling function for H_2 with updated H_2/H collisional rates

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ABSTRACT

The energy transfer among the components in a gas determines its fate. Especially at low temperatures, inelastic collisions drive the cooling and the heating mechanisms. In the early Universe as well as in zero- or low- metallicity environments the major contribution comes from the collisions among atomic and molecular hydrogen, also in its deuterated version. The present work shows some updated calculations of the H_2 cooling function based on novel collisional data which explicitely take into account the reactive pathway at low temperatures. Deviations from previous calculations are discussed and a multivariate data analysis is performed to provide a fit depending on both the gas temperature and the density of the gas.

Key words: Physical data and processes: molecular data, molecular processes. Stars: early-type. Cosmology: early universe.

1 INTRODUCTION

The thermal evolution of an interstellar cloud with primordial composition is deeply driven by the collisional and radiative processes occuring in the medium. In order to be properly described, it is essential not only to correctly model the dynamics but also to provide a complete description of the time variation of the gas temperature. To address this need, it is firstly required to identify the possible cooling mechanisms in the intergalactic medium (IGM); secondly, the models seek for functions that can be easily adopted in the models to reproduce each of the heating/cooling channels. In the context of IGM simulations and low metallicity interstellar medium (ISM) several works have been produced adopting this workflow(e.g., Black 1981; Shapiro & Kang 1987; Cen 1992; Glover & Jappsen 2007; Glover & Abel 2008; Glover & Savin 2009; Glover 2015); the same holds in the case of early Universe chemistry (Galli & Palla 2013), where the system is mainly consisting on hydrogen and helium. Mechanical ways of energy exchange are found in shocks and turbulence (e.g., Johnson & Bromm 2006; Kazandjian et al. 2016a; Kazandjian et al. 2016b; Vasiliev & Shchekinov 2017). The most relevant coolants at low temperatures are metals and molecules, both in gas phase and as dust in the intergalacting and in the interstellar medium. According to the radiation field in which the gas and the dust is embedded, heating mechanisms should be also taken into account in the thermal balance (e.g., Shchekinov & Vasiliev (2017)). On cosmological scales, the presence of even small traces of metals can determine a different fate in terms of masses of the first stars because of the line cooling (e.g., Bromm & Loeb 2003; Yoshida et al. 2006); gravitational instabilities are expected in the case of increasing metallicity content (Tanaka & Omukai 2014), together with thermal instabilities (Inoue & Omukai 2015). Indeed, the original gravitationally collapsing cloud can fragment or keep accreting according to the thermal conditions present in the gas (Omukai 2000; Latif et al. 2016). At the limit, the presence of coolant agents (both atomic and molecular) and a radiation field which has an intensity below the critical value can allow for the formation of supermassive black holes via direct accretion (e.g., Haiman et al. 1996; Sugimura et al. 2016). In the absence of heavier elements like carbon and oxygen (and the consequent possibility to form molecules like CO) the only way to cool the gas down to temperatures below few hundreds Kelvin is through rovibra-

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tional transitions of H_2 and its isotopic variants, the latter allowing to cool the gas even at temperatures below 100 K. For this reason, the description of the energy transfer associated with the H_2 line cooling deserves to be rigorously described, also by adopting the most complete data for each of the possible collisional partners. Specifically, in this paper, the case of the inelastic collisions of H_2 with atomic hydrogen is studied, explicitely introducing the reactive channel. The work is organized as follows: in Section 2 the basic concepts of the collisional pathways in the H_3 system are provided, together with the quantum mechanical methods adopted in the calculation of the cross-sections and the equation for the calculation of the cooling function. The kinetic model adopted and the chemical pathways included are also described; in Section 3, the results are reported. Moreover, a regression analysis of the data obtained for the cooling function is performed to derive a multivariate dependence of the cooling function on the gas temperature and density.

2 METHODS AND EQUATIONS.

In order to describe the time evolution of the level population for a N-levels system, the rate equation for each level should be provided. In the high density regime, the levels are distributed according to Maxwell-Boltzmann (e.g., Coppola et al. (2011a)). This hypothesis is in general not valid and the level population can be found by explicitely solving the rate equations which derive from the chemical processes introduced in the kinetics. In order to find the level population, two general approaches are usually adopted: on one hand, the time evolution of the levels population $\mathbf{x}$ can be found by solving the resulting system of ODEs Coppola et al. (2011b); Longo et al. (2011); otherwise, it can be assumed that the level population is in steady-state Martin et al. (1996); Tiné et al. (1998); Coppola et al. (2012). The calculations reported in this paper have been performed using the second assumption, that corresponds to imposing that the time derivative of the rate equations is equal to 0:

$$\frac{dx_i}{dt} = 0, \quad \forall i. \tag{1}$$

At each temperature and density, the whole problem of finding the steady-state population can be translated into a linear system formalism. Let $\mathbf{M}$ be the matrix that, when multiplied by the column vector of the population densities $\mathbf{n}$, results in the right hand side of the system of ordinary differential equations; the rate equations can be written then as (Tiné et al. 1998):

$$\frac{d\mathbf{n}}{dt} = \mathbf{M} \cdot \mathbf{n} \tag{2}$$

Then, the level population derives from the chemical channels that most effectively redistribute them among the rovibrational manifold; the choice of such channels depends on the system of interest. The case reported in this paper corresponds to the typical freeze-out abundances that can be found in the early Universe chemistry. The H_2 collisional partners included are H, He and H^+; moreover, the formation and destruction pathways for the molecular hydrogen are the associative detachment of H and H^- and the dissociative attachment of H_2, respectively. Radiative transition are inserted and the data by Wolniewicz et al. (1998) have been adopted. The relative abundances of He and H^+ respect to H are 10^{-1} and 2×10^{-4}. The reaction rates included for the formation and destruction channels of H_2 have been taken from Coppola et al. (2011b) and Capitelli et al. (2007). The collisional data with He are fully available for the whole H_2 rovibrational manifold (F. Esposito, private communication and Celiberto et al. 2017). The collisional data for the system H $_2$-H^+ have been included using the fits provided by Gerlich (1990); transitions up to $(v = 0, j = 8)$ are therein reported. Finally, the reactive H_2-H collisions have been included; details on the adopted data are described in the following. According to the reactive data provided for H_2-H, the number of levels included in the present calculations is 55, that corresponds to $(v = 3, j = 18)$.

2.1 Updates collisional data: H_2–H reaction rates.

The modeling of accurate cooling functions relies on the calculations of H_2-H collisional rate coefficients. Such calculations are challenging since two processes are in competition during collisions between H_2 and H:
-the inelastic process:

$$H_2(v, j) + H' \rightarrow H_2(v', j') + H'$$

-the exchange process:

$$H_2(v, j) + H' \rightarrow H'H(v', j') + H$$

where v and j designates the vibrational and rotational level of H_2, respectively. This is explained by the reactive nature of the H_3 system. The obtention of accurate collisional data requires to consider simultaneously both processes during the calculations. In particular, the ortho–para-H_2 conversion can only occur through the hydrogen exchange channel.

Ro-vibrational relaxation of H_2 by H have been extensively studied using quasi-classical trajectory calculations (Mandy & Martin 1993, and references therein). Unfortunately, the inability of quasi-classical trajectory treatments to conserve the vibrational zero-point energy renders this method unreliable near reaction thresholds. Alternatively, Flower and co-workers (Wrathmall & Flower 2007; Wrathmall et al. 2007) computed ro-vibrational rate coefficients for temperatures ranging from 100 to 6000 K using a quantum close coupling approach neglecting the reactive channels arguing that reactivity is negligible for temperatures up to 6000 K. They did not consider the ortho–para-H_2 conversion process and neglect the vibrational relaxation that occur through the exchange process that is expected to be important even at low temperatures.

Hence, there were still a lack of highly accurate collisional data until we recently presented quantum mechanical calculations of cross sections for the collisional excitation of H_2 by H including the reactive channels (Lique et al. 2012; Lique et al. 2014; Lique 2015) using the state-of-the-art PES of Mielke et al. (2002). We refer the reader to these papers for full details on the scattering calculations. In summary, calculations were performed using the almost exact close coupling approach. New collisional data were obtained for the ro-vibrational relaxation of highly excited H_2 (with internal excitation up to $\simeq$ 22000 K) for temperatures ranging from 100 to 5000 K. The theoretical results were checked

against available experimental data and a good agreement was found for both ro- vibrational relaxation (Lique 2015) and ortho–para-H_2 conversion process (Lique et al. 2012).

The new results significantly differ from previous data widely used in astrophysical models (Wrathmall & Flower 2007; Wrathmall et al. 2007). Important deviations are observed at low temperatures for ro-vibrational transitions whereas, for pure rotational transitions, the mean deviations occur at high temperatures. These differences are principally due to the inclusion of the reactive channels in the scattering calculations.

2.2 Cooling function

The calculation of the cooling function requires information about the level population, computed at each gas temperature, and on the energy gaps and Einstein coefficients between the levels included in the model. In particular, for a generic molecule *mol*, the cooling function in defined as:

$$n_{mol}\Lambda = \sum_j \sum_{i<j} n_j A_{ji} \beta_{ji} (E_j - E_i) \qquad (3)$$

with Λ in erg s^{-1}, n_{mol} the density of the molecule, n_j the density for the j^{th} level and β_{ji} is the escape probability of the emitted photon. The assumption under which the calculations here presented are performed is that the medium is optically thin; in this case, all the emitted photons can escape from the medium without being re-absorbed and in Eq. 3 the term β_{ji} is equal to 1. The calculation of the cooling function has been performed using the code `FRIGUS` developed by Kazandjian & Coppola (2019). No assumptions have been adopted on the level population between ortho- and para-H_2, that have been explicitely calculated according to the steady-state approximation and detailed balance between radiative and collisional rates. Stimulated process are included in `FRIGUS` where a Planckian radiation field has been implemented by default to mimic the cosmic microwave background at a certain redshift z; however, the calculations reported in this work have been performed for a radiation temperature equal to zero. The Einstein coefficients have been calculated by Wolniewicz et al. (1998); the energy levels used have been taken from the UGA - Molecular Opacity Project Database and the collisional reaction rates adopted are the ones computed by Lique (2015).

3 RESULTS

3.1 Cooling function

In Fig. 1 the cooling function obtained adopting the updated collisional reaction rates by Lique (2015) is reported as a function of the kinetic temperature for several values of the gas density (black continuous curves, from the low to the high density limit, corresponding to the lower and upper curves, respectively). The dependence from the density follows what shown by Lipovka et al. (2005) for HD: the curves tend to converge for high values of density to the LTE cooling function, i.e. to the cooling function that can be obtained by assuming that the level population is described by a Maxwell-Boltzmann distribution for the energy levels.

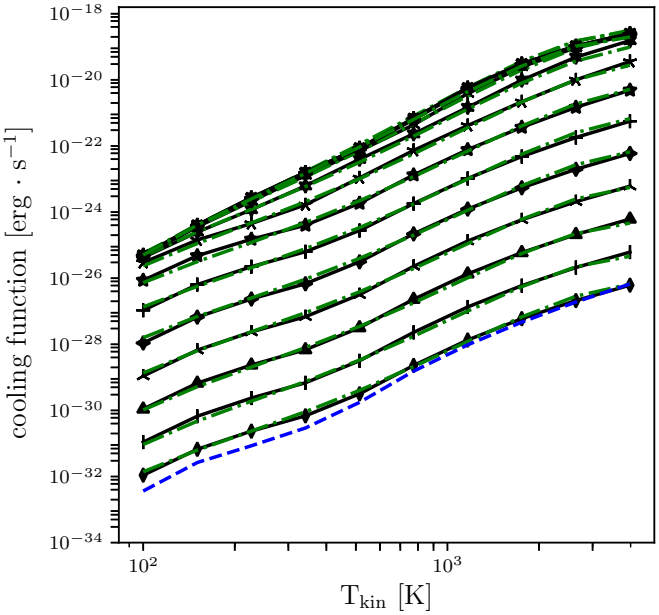

Figure 1. Cooling functions at different densities adopting the new data (Lique et al. 2012; Lique et al. 2014; Lique 2015) and the software `FRIGUS` (black continuous curves). From bottom to top, the corresponding densities are: 10^2 m^{-3}, 10^3 m^{-3}, 10^4 m^{-3}, 10^5 m^{-3}, 10^6 m^{-3}, 10^7 m^{-3}, 10^8 m^{-3}, 10^9 m^{-3}, 10^{10} m^{-3}, 10^{11} m^{-3}, 10^{12} m^{-3}, 10^{13} m^{-3}, 10^{14} m^{-3} As a comparison, the fit provided by Glover & Abel 2008 is also shown (blue dashed curve). The dash-dotted curves correspond to the fit provided in the present paper; see text for details.

This case corresponds to a gas in which the fractional abundances of internal rovibrational levels is thermalized, while in the more general case this situation is not necessarly satisfied.

In the same figure, the most recent fit for H_2/H cooling by Glover & Abel (2008) is also reported, which is based on the data by Wrathmall & Flower (2007). At low temperatures T$\sim$ 100 K, deviations up to an order of magnitude can be appreciated. Together with the different collisional data implemented, such a difference may be explained assuming that their fit has been performed assuming an ortho-to-para ratio 3:1. In the absence of a full state-to-state description of the kinetics of rovibrational levels, assuming an ortho-to-para is the only way to proceed in the calculations. Moreover, collisional processes with other atomic or molecular partners may allow to reach the statistical ortho-to-para in a faster way, allowing to confidently use the 3:1 value in the simulations. For example, it is well known that collision with protons are very effective in the ortho-to-para conversion of H_2, as reported by Gerlich (1990) and recently confirmed by Grozdanov (2014). However, as also acknowledged in the introduction of the work by Glover & Abel (2008), deviations from the 3:1 ortho-to- para ratio are expected at low temperatures, as explicitely captured by performing the calculations using `FRIGUS`). The ideal procedure would then prescribe to solve the kinetics of rovibrational level of H_2 in each particular case and to compute the actual level population and cooling *on-the-fly*.

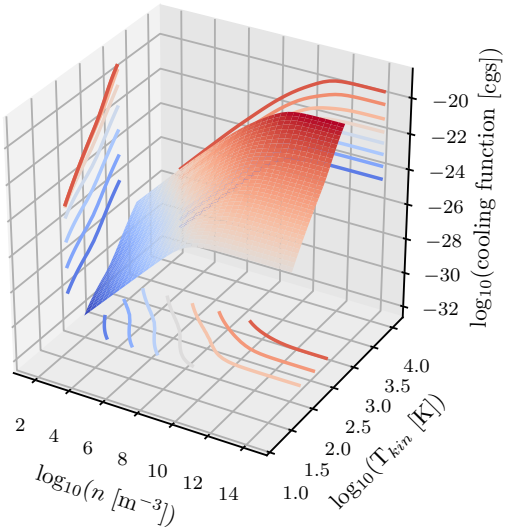

Figure 2. 3D rendering of the cooling function at different densities and kinetic temperatures using `FRIGUS` (Kazandjian & Coppola 2019). SI units are used.

In Fig. 2 a 3D-rendering of the cooling functions surface is reported with a colour code to distinguish more easily the values of the independent variables and the cooling functions themselves.

3.2 Fit

In order to allow for a faster usage of the calculated cooling function at several kinetic temperatures and densities, we provide the users with a fitted expressions for the cooling functions; the same expression used by Lipovka et al. (2005) in the case of HD is used:

$$log10(\Lambda) = \sum_{l,m=0}^{4} D_{lm}(log_{10}T)^l(log_{10}n)^m \qquad (4)$$

where the numerical values of the logarithms are taken expressing the temperature in Kelvin and the density in cgs units; the resulting cooling function Λ has units erg $\times$ s^{-1}. The parameters are provided in Table 1. In Fig. 1 the comparison between the computed data (black full) and the fit (green dashed curves) is also reported, showing very small errors (the largest being $\sim 10^{-3}$).

4 CONCLUSIONS

Thanks to available updated cross-sections for the inelastic processes $H_2(v,j)$+H $\rightarrow$ $H_2(v',j')$+H (Lique 2015) and the state-to-state software `FRIGUS` (Kazandjian & Coppola 2019), a new cooling function depending both on gas temperature and density has been evaluated, which include the rovibrational levels up to ($v = 3, j = 18$). The inclusion of reactive channels increased the cooling effect at high temperatures, together with a larger set of included rovibrational levels in the energy exchange evaluation

For facilitating the usage of these results, a multivariate analysis is performed and the resulting fit is reported together with the parameters in Sec. 3.2. The computation has been performed for radiation temperature equal to zero, to compare the results with previous calculations; however, if needed, the software `FRIGUS` can be used to recover the cooling function at different radiation temperature (i.e. different epochs in the case of simulations describing early Universe chemistry or early star formation).

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	m = 0	m = 1	m = 2	m = 3	m = 4
l = 0	-1.07761178e+02	+8.50704285e+00	-3.08850636e-01	-3.97357274e-01	+3.65589231e-02
l = 1	+1.17901741e+02	-1.09489742e+01	+2.51708582e-01	+5.47452438e-01	-4.89055533e-02
l = 2	-6.61721218e+01	+5.95232129e+00	-1.10639748e-01	-2.92423859e-01	+2.57375696e-02
l = 3	+1.67152116e+01	-1.43513388e+00	+2.84953800e-02	+7.02040444e-02	-6.18478233e-03
l = 4	-1.55475014e+00	+1.29639563e-01	-3.13943372e-03	-6.36261310e-03	+5.65797161e-04

Table 1. Parameters for the cooling function fit as reported in Sec. 3.2; Λ has units erg $\times$ s^{-1}. These parameters are valid in the density range [10^2-10^{14}] m^{-3} and temperature range [100-4000] K.

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