ON THE RELATIVE ABUNDANCE OF LiH AND LiH\(^+\) MOLECULES IN THE EARLY UNIVERSE: NEW RESULTS FROM QUANTUM REACTIONS

Stefano Bovino\(^1\), Mario Tacconi\(^1\), Franco A. Gianturco\(^1\), Daniele Galli\(^2\), and Francesco Palla\(^2\)

\(^1\) Department of Chemistry and CNISM, The University of Rome “Sapienza,” Ple A. Moro 5, 00185 Roma, Italy; fa.gianturco@caspur.it
\(^2\) INAF-Osservatorio Astrofisico di Arcetri, Largo E. Fermi 5, 50125 Firenze, Italy

Received 2010 December 16; accepted 2011 February 17; published 2011 March 30

ABSTRACT

The relative efficiencies of the chemical pathways that can lead to the destruction of LiH and LiH\(^+\) molecules, conjectured to be present in the primordial gas and to control molecular cooling processes in the gravitational collapse of the post-recombination era, are revisited by using accurate quantum calculations for the several reactions involved. The new rates are employed to survey the behavior of the relative abundance of these molecules at redshifts of interest for early universe conditions. We find significant differences with respect to previous calculations, the present ones yielding LiH abundances higher than LiH\(^+\) at all redshifts.

Key words: astrochemistry – early universe – evolution – molecular processes

1. INTRODUCTION

The suggestion that chemical processes involving lithium could play a role in the evolution of the early universe in the post-recombination era has been put forward several years ago (Lepp & Shull 1983; Stancil et al. 1996, hereafter SLD96; Galli & Palla 1998, hereafter GP98), starting from the consideration that Li is produced a few minutes after the big bang and the formation of other light atoms such as H, D, and He (Wagoner et al. 1967; Peebles 1993). The fractional abundances of these elements are sensitive to the baryon density of the universe and set constraints on its actual value (Cyburt et al. 2008). As the universe expanded, its radiation temperature decreased and the atomic ions originating from the above elements gave rise to neutral atoms by recombination with electrons, thus initiating the formation of molecular species by radiative association: H\(_2\), HD, and LiH. The latter molecule, because of its large dipole moment and low ionization potential, may induce spatial and/or spectral distortions in the cosmic background radiation (CBR), as originally suggested by Dubrovich (1993) and as experimentally surmised by the pioneering work of Maoli et al. (1994). Eventually, during the gravitational collapse leading to the formation of the first stars, the low-excitation threshold and the efficient radiative decay along the rovibrational manifold are additional properties that could favor the role of LiH and LiH\(^+\) as molecular coolants of the primordial gas (Bougleux & Galli 1997, hereafter BG97). The nonequilibrium level population in the presence of a different gas and radiation temperature may have a possible signature in protogalactic clouds, imprinting small fluctuations in the CBR spectrum (Schleicher et al. 2008), as we shall further discuss in our conclusions.

The chemistry of Li in the early universe has been discussed in the past, reaching contrasting conclusions (see, e.g., SLD96; BG97; GP98; Vonlanthen et al. 2009). Of critical relevance is the uncertainty in the knowledge of reliable reaction rates for the destruction of LiH and LiH\(^+\) molecules via strongly exothermic reactions without entrance barriers:

\[
\text{LiH} + \text{H} \rightarrow \text{Li} + \text{H}_2, \quad (1)
\]

\[
\text{LiH} + \text{H}^+ \rightarrow \text{Li} + \text{H}_2^+, \quad (2)
\]

and

\[
\text{LiH}^+ + \text{H} \rightarrow \text{Li}^+ + \text{H}_2. \quad (3)
\]

Therefore, it is an accurate knowledge of the reaction rates for the above processes, at low-redshift values that can ultimately tell us what the end role of the LiH/LiH\(^+\) systems could be as efficient coolants under early universe conditions. The task of the present work is to show that the reaction rates recently determined from fully ab initio quantum methods (Bovino et al. 2009, 2010a, 2010b), which also employ accurate interaction forces between partners, have a significant impact on the evolution of LiH and LiH\(^+\) during the post-recombination era of the early universe. We shall further show that a more realistic computational description of the rates for a neutralization process

\[
\text{LiH}^+ + e^- \rightarrow \text{Li} + \text{H} \quad (4)
\]

could substantially change the relative abundance of the ionic molecular species.

This paper is organized as follows: the details of the quantum methods for the new chemical reaction rates are given in Section 2, while Section 3 reports the list of considered reactions and describes the equations controlling the evolution of the gas temperature. In Section 4 we present the fractional abundances and an analysis of their behavior, while Section 5 summarizes our present conclusions.

2. THE QUANTUM REACTIVE CALCULATIONS

The study of the chemical evolution of the main species of the primordial gas requires accurate rate coefficients for the most important destruction reactions. In previous works, the Langevin approximation for barrierless reactions has been the main method used to obtain the rate coefficients for those reactions. In the last decade, with the development of more realistic methods for reaction processes, a great deal of work has been done to study reactions (1), (2), and (3). For instance, time-dependent (Bulut et al. 2008; Defazio et al. 2005) and quasi-classical trajectory (Pino et al. 2008; Dunne et al. 2001) calculations have been reported, and some of the calculated rates have been included in the abundance calculations of Lepp et al. (2002). However, most of these calculations are restricted to a narrow range of energies or are limited to the high
energy regime. Therefore, the main improvement of the present calculations has been the use of new, very accurate potential energy surfaces (Martinazzo et al. 2003a, 2003b; Wernli et al. 2009) combined with accurate quantum reactive calculations. The quantum methods range from the fully ab initio coupled reactive scattering methods (see Section 2) to the use of a negative imaginary angular momentum, \( J_a \), and \( k^2_a \) is the wave vector defined as

\[ k^2_a = \frac{2\mu}{\hbar^2}(E - \varepsilon_a), \]

and \( \varepsilon_a \) is the \( a \)-channel energy. Rate coefficients are computed by averaging the appropriate reactive cross sections over a Boltzmann distribution of velocities for the incoming atom:

\[ k(T_g) = \frac{(8\pi \hbar^2 \mu / k_B T_g)^{1/2}}{(k_B T_g)^2} \int_0^\infty \sigma_{a \to all}(E) \exp(-E/k_B T_g) E dE, \]

where \( T_g \) is the gas temperature, \( k_B \) is the Boltzmann constant, and \( \mu \) is the reduced mass of the system. The newly computed rate coefficients for reactions (1), (2), and (3) are reported in Bovino et al. (2009, 2010a, 2010b) and shown in Figure 1. The corresponding temperature-dependent fits are given in Table 1, along with all the reactions rates for the Li species employed in the present work.

3. THE CHEMICAL NETWORK AND THE EVOLUTIONARY MODELING

The evolution of the pregalactic gas is considered in the framework of a Friedmann cosmological model and the primordial abundances of the main gas components are taken from the standard big bang nucleosynthesis results (Smith et al. 1993). The numerical values of the cosmological parameters used in the calculation are obtained from WMAP5 data (Komatsu et al. 2009) and are listed in Table 2 (see Coppola et al. 2011 for details).

In order to calculate the abundances of LiH and LiH*, a set of differential coupled chemical rate equations of the form

\[ \frac{d n_i}{dt} = k_{\text{form}} n_j n_k - k_{\text{dest}} n_i + \cdots \]

has been solved. In Equation (8), \( k_{\text{form}} \) and \( k_{\text{dest}} \) are the formation and destruction reaction rates as listed in Table 1, and \( n_i \) is the number density of the reactant species \( i \). The evolution of the gas temperature \( T_g \) is governed by the equation (see, e.g., GP98)

\[ \frac{dT_g}{dt} = -2T_g \frac{R}{\dot{R}} + \frac{2}{3k n} \left[ (\Gamma - \Lambda)_{\text{Compton}} + (\Gamma - \Lambda)_{\text{mol}} \right], \]

and via excitation and de-excitation of molecular transition,

\[ (\Gamma - \Lambda)_{\text{mol}} = \sum_k n_k \sum_{i<j} (x_i C_{ij} - x_j C_{ji}) \hbar \nu_{ij}, \]

where \( C_{ij} \) and \( C_{ji} \) are the collisional excitation and de-excitation coefficients and \( x_i \) are the fractional level populations; for more details of this model, see BG97 and GP98. The radiation temperature is \( T_r(z) = T_0(1 + z) \), where \( T_0 \) is the present-day CBR temperature. The chemical/thermal network is then completed by the rate equation for the redshift

\[ \frac{dt}{dz} = \frac{1}{(1 + z) H(z)}, \]

where

\[ H(z) = H_0 \sqrt{\Omega_r (1 + z)^4 + \Omega_m (1 + z)^3 + \Omega_k (1 + z)^2 + \Omega_\Lambda}. \]

Here, \( H_0 \) is the Hubble constant and \( \Omega_r, \Omega_m, \Omega_k, \Omega_\Lambda \) are density parameters. The density \( n(z) \) of baryons at redshift \( z \) is

\[ n(z) = \Omega_b n_{c}(1 + z)^3, \]

with \( n_{c} = 3 H_0^2 / (8\pi G m_{H}) \) being the critical density. The calculations have been carried out from \( z = 10^4 \) down to \( z = 1 \) and are discussed in the next section.
4. RESULTS AND DISCUSSION

As discussed in the Introduction, one of the novelties of the present work is the use, for some of the most important chemical processes, of rates obtained from accurate quantum calculations and not from qualitative estimates. It is therefore important for the reactions involving LiH/LiH$^+$ to recall the chemical processes, of rates obtained from accurate quantum calculations of Bovino et al. (2009) indicate a variation over the same range of temperatures. Finally, the quantum rates associated with the destruction of LiH$^+$ by the surrounding hydrogen gas (bottom panel) confirm the weak temperature dependence reported earlier (Lepp et al. 2002), although they turn out to be about a factor of four larger than the estimate of SL96. Once the new quantities are employed within the evolutionary scheme outlined in Section 3, they yield a new set of production/destruction rates of LiH and LiH$^+$ as a function of redshift, as shown in Figures 2 and 3.

4.1. LiH Chemistry

The various curves shown in Figure 2 follow the notation given in Table 1 to the most relevant processes: those labeled as $p_1, \ldots, p_4$ (solid lines) refer to the different reactions leading

Table 1

| No. | Figure Label | Reaction | Rate (cm$^3$ s$^{-1}$ or s$^{-1}$) | Notes | Reference |
|-----|-------------|----------|-----------------------------------|-------|-----------|
| (1) | $p_1$       | Li($^7\text{p}$) + H $\rightarrow$ LiH + hν | $2.0 \times 10^{-16} T_e^{0.18} \exp(-T_e/5100)$ | $A^1\Sigma^+ \rightarrow X^1\Sigma^+$, quantal calc. | (a) |
| (2) | $p_1$       | Li($^7\text{p}$) + H $\rightarrow$ LiH + hν | $1.9 \times 10^{-14} T_e^{-0.34}$ | $B^1\Pi \rightarrow X^1\Sigma^+$, quantal calc. | (a) |
| (3) | $p_2$       | Li + H $\rightarrow$ LiH + hν | $4.0 \times 10^{-20} \exp(-T_e/4065 + (T_e/13193)^3)$ | Quantal calc. | (b),(c),(d) |
| (4) | $p_3$       | Li + H$^+$ $\rightarrow$ LiH + e | $4.0 \times 10^{-10}$ | Estimate | (e) |
| (5) | $p_4$       | Li + H$^+$ $\rightarrow$ LiH$^+$ + hν | $5.3 \times 10^{-14} T_e^{-0.49}$ | Quantal calc. | (c),(d) |
| (6) | $p_5^*$     | Li + H$^+$ $\rightarrow$ Li$^+$ + H$^+$ | $2.5 \times 10^{-40} T_e^{-3.9} \exp(-T_e/1210)$ | Quantal calc. | (f) |
| (7) | $p_6^*$     | Li + H$^+$ $\rightarrow$ Li$^+$ + H + hν | $1.7 \times 10^{-11} T_e^{-0.651} \exp(-T_e/282000)$ | Quantal calc. | (g) |
| (8) | $p_7^*$     | Li + e $\rightarrow$ Li$^+$ + hν | $6.1 \times 10^{-17} T_e^{-0.58} \exp(-T_e/17200)$ | Det. bal. applied to (27) | |
| (9) | $p_8^*$     | Li + H$^+$ $\rightarrow$ LiH + H$^+$ | $6.3 \times 10^{-10} \exp(-2553/T_e)$ | $T_e < 500$, quantal calc. | (i) |
| (10)| $p_9^*$     | Li$^+$ + H $\rightarrow$ LiH$^+$ + hν | $1.4 \times 10^{-20} T_e^{-0.9} \exp(-T_e/7000)$ | Quantal calc. | (c),(d) |
| (11)| $p_9^*$     | Li$^+$ + e $\rightarrow$ Li + hν | $1.036 \times 10^{-11} [T_e/107.7]^{-0.6612} \exp(-1 + \sqrt{T_e/(1.177 \times 10^{13} 3388)}-1)$ | Quantal calc. | (k) |
| (12)| $p_9^*$     | Li$^+$ + H$^+$ $\rightarrow$ Li + H | $6.3 \times 10^{-9} T_e^{-1/2} (1 + T_e/14000)$ | Landau-Zener approx. | (l) |
| (13)| $p_4$       | Li$^+$ + H $\rightarrow$ LiH + e | $4.0 \times 10^{-10}$ | Estimate | (e) |
| (14)| $p_4$       | Li$^+$ + H$^+$ $\rightarrow$ LiH + e | $2.3 \times 10^{-6} T_e^{-1/2}$ | Landau-Zener approx. | (l) |
| (15)| $d_1$       | LiH + H $\rightarrow$ Li + H$_2$ | $2.0 \times 10^{-12} T_e^{0.046} \exp(-T_e/1200)$ | Quantal calc. | (m) |
| (16)| $d_3$       | LiH + H$^+$ $\rightarrow$ Li + H$_2^+$ | $2.9 \times 10^{-10} T_e^{0.56}$ | Quantal calc. | (n) |
| (17)| $d_3^*$, $d_4$ | LiH + H$^+$ $\rightarrow$ LiH$^+$ + H | $1.0 \times 10^{-9}$ | Quantal calc. | (o) |
| (18)| $d_4$       | LiH + H$^+$ $\rightarrow$ Li$^+$ + H$^+$ | $1.0 \times 10^{-9}$ | Estimate | (e) |
| (19)| $d_5$       | LiH$^+$ + H$^+$ $\rightarrow$ Li$^+$ + H$_2^+$ | $8.7 \times 10^{-10} T_e^{0.046} \exp(T_e/5.92 \times 10^3)$ | Quantal calc. | (p) |
| (20)| $d_5$       | LiH$^+$ + H $\rightarrow$ Li + H$^+$ | $9.0 \times 10^{-10} \exp(-66400/T_e)$ | Estimate | (e) |
| (21)| $d_5$       | LiH$^+$ + H $\rightarrow$ LiH$^+$ | $1.0 \times 10^{-11} \exp(-67900/T_e)$ | Estimate | (e) |
| (22)| $d_5^*$     | LiH$^+$ + e $\rightarrow$ Li$^+$ + e | $3.9 \times 10^{-6} \exp(-T_e/1200)$ | Quantal calc. | (q) |
| (23)| $d_1$       | LiH + hν $\rightarrow$ Li + H | Det. bal. applied to (3) |
| (24)| $d_1$       | LiH$^+$ + hν $\rightarrow$ Li$^+$ + H$^+$ | Det. bal. applied to (10) |
| (25)| $d_2$       | LiH + H$^+$ $\rightarrow$ Li + H$^+$ | Det. bal. applied to (5) |
| (26)| $d_2$       | Li + hν $\rightarrow$ Li$^+$ + e | Det. bal. applied to (11) |
| (27)| $d_2$       | Li$^+$ + hν $\rightarrow$ Li + e | Quantal calc. | (h) |
| (28)| $d_2$       | LiH$^+$ + hν $\rightarrow$ Li$^+$ + e | Det. bal. applied to (1), (2) |

Note. Labels in the second column refer to Figures 2 and 3.

References. (a) Ganturco & Gori Giorgi 1996; (b) Bennett et al. 2003; 2008; (c) Dalgoano et al. 1996; (d) Ganturco & Gori Giorgi 1997; (e) Stancil et al. 1996; (f) Kimura et al. 1994; (g) Stancil & Zygelman 1996; (h) Ramsbottom et al. 1994; (i) Bulut et al. 2009; (j) Pino et al. 2008; (k) Verner & Ferland 1996; (l) Croft et al. 1999; (m) Bovino et al. 2009; (n) Bovino et al. 2010b; (o) Bulut et al. 2008; (p) Bovino et al. 2010a; (q) Čurik & Greene 2007, 2008.
respectively. See the text for details.

Solid and dashed curves represent production and destruction processes, respectively. A look at the figure allows one to make the following comments.

1. The production by radiative recombinations from the \( \text{Li}(^2 P) \) state \( (p_1) \) clearly dominates at high redshifts, while the production by recombinations from the \( \text{Li}(^2 S) \) state \( (p_2) \) becomes the dominant route from \( z \approx 800 \) down to \( z \approx 80 \). Then, the channel of recombinations driven by electron attachment \( (p_4) \) takes over. However, we must note that the latter rate is not known from quantum calculations, but only estimated by SLD96, together with the estimates of LiH formation from H\(^+\) (SLD96).

2. At the highest redshifts, the destruction channel is dominated by photodissociation \( (d_1) \), a rate estimated from the detailed balance of process \( (p_2) \), while at lower \( z \) values \( (z \lesssim 300) \) the collisional process of reactive destruction discussed earlier \( (d_2) \) takes over and dominates the whole destruction channel down to the lowest redshifts. The same reactive process with protons \( (d_3) \) is seen to be less important, although larger than previous estimates \( (d_4) \).

In conclusion, the above data indicate that the radiative photodissociation from the \( n = 25 \) level of Li is the most significant formation path, while the collisional destruction by H \( (d_3) \) overcomes production over the whole range of redshifts below 300.

4.2. LiH\(^+\) Chemistry

Figure 3 shows the processes leading to the formation and the destruction of \( \text{LiH}^+ \), labeled as \( p_1, \ldots, p_4 \) and \( d_1, \ldots, d_4 \) as in Table 1. As clearly shown by the figure, the radiative association processes \( (p_1 \) and \( p_2 \) are seen to dominate the formation of \( \text{LiH}^+ \) over a very broad range of redshifts. The association involving the Li ion \( (p_1) \) is the major pathway down to about \( z \approx 700 \), when the reaction of \( \text{H}^+ \) with neutral Li \( (p_2) \) takes over and becomes dominant by several orders of magnitude over the rates of the charge-exchange reaction \( (p_3) \) estimated by SLD96.

As for the destruction processes for \( \text{LiH}^+ \), one sees that the photodissociation \( (d_2) \) is the dominant destruction path of the ionic molecule, due to its small dissociation energy value. Furthermore, the dominant dissociation channel comes from \( \text{Li}^+ \) production \( (d_3) \), while the one yielding \( \text{H}^+ \) \( (d_4) \) is relevant only at the highest redshifts. The electron-induced dissociation \( (d_4) \) was earlier based on simple estimates from SLD96 while now we have included the more accurate quantum calculations from Čurík & Greene (2007, 2008) which yield much larger rates. It turns out to be important only at low redshifts. On the other hand, the chemical paths which involve the reactions that destroy \( \text{LiH}^+ \) \( (d_4) \) are seen to be indeed the most important processes around \( z \approx 40 \) while becoming less efficient than the \( d_3 \) process below \( z \approx 10 \). The electron-assisted dissociation of \( \text{LiH}^+ \) \( (d_1) \) is therefore important only at the lowest redshifts.

In summary, the ionic formation is dominated by the radiative association of Li with \( \text{H}^+ \) over a very broad range of redshifts, while destruction by photodissociation prevails at larger redshift and chemical destruction \( (d_1) \) dominates at lower redshifts. However, down to \( z \approx 1 \) the dissociative neutralization \( (d_1) \) is markedly dominant.
according to Spergel et al. (2007).

The dotted lines at $z = 11$ and $z = 7$ indicate the approximate redshifts at which reionization of the primordial gas starts ($z \sim 11$) and is completed ($z \sim 7$), according to Spergel et al. (2007).

4.3. Chemical Evolution

The new evolution of relative abundances of atomic and molecular species involving Li is displayed in Figure 4, comparing the earlier results obtained with the chemical network of GP98 (dashed lines) and the present results (solid lines) which employ the new quantum rates. The main results are the following.

1. The temperature dependence of the quantum rates, shown by the data of Figure 1, is clearly reflected in the molecular abundances of LiH at redshifts below $z \sim 300$. The rapid rise of LiH at $z \sim 300$ found by GP98 is no longer seen owing to the increased destruction rate of channel (1). The rise at $z \sim 100$ is due to the importance of LiH formation by Li− that persists at all redshifts together with the radiative association of Li with H. This is drastically different from the behavior found by GP98 where the constant value of the rate for reaction (1) caused the steady drop of LiH. The final ($z = 0$) value of LiH is $\sim 7 \times 10^{-18}$ with an increase of a factor of $\sim 70$ relative to GP98.

2. Due to the differences in behavior shown by the cross sections in Figure 1, the ionic partner, LiH+, behaves differently at $z \lesssim 30$. First, the increased efficiency of LiH+ destruction (reaction (3); rate $d_1^+$) limits the sharp rise in abundance at $z \sim 20$. Then, the gentle decline below $z \sim 5$ is due to the efficiency of electronic recombination (rate $d_{7}^+$). The new final abundances of LiH+ (solid line) is now smaller than earlier estimates of GP98 by a factor of $\sim 20$.

The scenario emerging from the above calculations therefore indicates that in the regions of redshift below $z \sim 30$, LiH remains the more abundant species compared to LiH+, but only by a factor of $\sim 2$--7. The two molecular abundances, on the other hand, reach the largest values for $z \lesssim 10$, remaining both fairly small (LiH $\sim 10^{-17}$, LiH+ $\sim 10^{-18}$) and hard to detect.

5. CONCLUSIONS

Building upon recent quantum reactive calculations (Bovino et al. 2009, 2010a, 2010b) involving the chemical evolution of LiH/LiH+ molecules within the expected conditions in the early universe, the present work has revisited the analysis of all the dynamical processes that are known to significantly contribute to the production/destruction of the lithium-containing molecules. We have employed as many results as possible from calculations based on ab initio methods, both for the interaction forces and the quantum dynamics, resorting to estimates only for a few of the considered processes.

One of the main results from the quantum reactive calculations is that two of the important rates exhibit a temperature dependence that was not present in the earlier estimates.

The results for the abundance of LiH indicate that this molecule is now much more likely to have survived at low redshift, since its fractional abundance, albeit still fairly small, goes up by a factor of $\sim 70$ compared to previous estimates. However, it becomes smaller by nearly the same amount for $z > 300$.

The fractional abundance of LiH+ only becomes significant in the low-redshift region of $z \lesssim 30$ and shows a reduced value of the relative abundance by about one order of magnitude with respect to the earlier estimates. The comparison between the specific fractional abundances of the two species now indicates that the neutral molecule is likely to be more abundant than the ionic species and that their ratio in the region of small redshift increases up to a factor of seven down to $z \sim 1$. Unlike previous estimates that predicted a difference at low-$z$ of about two orders of magnitude in favor of LiH+, the new calculations find more comparable abundances of LiH and LiH+. Furthermore, we find that the neutral molecule, in spite of a large dilution at the low redshifts, should be more amenable to experimental observation (e.g., Persson et al. 2010) than its ionic counterpart.

Finally, given the recent studies (e.g., see Zaldarriaga & Loeb 2002) on the possible detection, within the microwave background anisotropies, of the earlier imprint from the recombination history of lithium, the present results strongly suggest that such anisotropies could be amenable to observation due to the changed optical depth induced by the changes in lithium abundances.

We thank the CINECA and CASPUR consortia for providing us with the necessary computational facilities and the University of Roma “Sapienza” for partial financial support.

REFERENCES

Bennett, O. J., Dickinson, A. S., Leininger, T., & Gadéa, F. X. 2003, MNRAS, 341, 361
Bennett, O. J., Dickinson, A. S., Leininger, T., & Gadéa, F. X. 2008, MNRAS, 384, 1743
Bougie, E., & Galli, D. 1997, MNRAS, 288, 638 (BG97)
Bovino, S., Stoecklin, T., & Gianturco, F. A. 2010a, ApJ, 708, 1560
Bovino, S., Tacconi, M., Gianturco, F. A., & Stoecklin, T., 2010b, ApJ, 724, 106
Bovino, S., Wernli, M., & Gianturco, F. A. 2009, ApJ, 699, 383
Bulut, N., Castillo, J. F., Aoiz, F. J., & Banares, L. 2008, Phys. Chem. Chem. Phys., 10, 821
Bulut, N., Castillo, J. F., Banares, L., & Aoiz, F. J. 2009, J. Phys. Chem. A, 113, 14657
Coppola, C. M., Longo, S., Capitelli, M., Palla, F., & Galli, D. 2011, ApJS, 193, 7
Croft, H., Dickinson, A. S., & Gadéa, F. X. 1999, MNRAS, 304, 327
Čurík, R., & Greene, C. H. 2007, Phys. Rev. Lett., 98, 173201
Čurík, R., & Greene, C. H. 2008, J. Phys.: Conf. Ser., 115, 012016
Cyburt, R. M., Fields, B. D., & Olive, K. A. 2008, J. Cosmol. Astropart. Phys., JCAP11(2008)012
Dalgarno, A., Kirby, K., & Stancil, P. C. 1996, ApJ, 458, 397
Defazio, P., Petrongolo, C., Gamallo, P., & González, M. 2005, J. Chem. Phys., 122, 214303
Dubrovich, V. K. 1993, Astron. Lett., 19, 53
Dunne, L. J., Murrell, J. N., & Jenner, P. 2001, Chem. Phys. Lett., 336, 1
Galli, D., & Palla, F. 1998, A&A, 335, 403 (GP98)
Gianturco, F. A., & Gori Giorgi, P. 1996, Phys. Rev. A., 54, 1
Gianturco, F. A., & Gori Giorgi, P. 1997, ApJ, 479, 560
Kimura, M., Dutta, C. M., & Shimakura, N. 1994, ApJ, 430, 435
Komatsu, E., et al. 2009, ApJS, 180, 330
Lepp, S., & Shull, J. M. 1983, ApJ, 270, 578
Lepp, S., Stancil, P. C., & Dalgarno, A. 2002, J. Phys. B: At. Mol. Opt. Phys., 35, R57
Maoli, R., Melchiorri, F., & Tosti, D. 1994, ApJ, 425, 372
Martínez-Pinedo, G., Bodo, E., Gianturco, F. A., & Raimondi, M. 2003a, Chem. Phys., 287, 335
Martínazzò, R., Tantardini, G. F., Bodo, E., & Gianturco, F. A. 2003b, J. Chem. Phys., 119, 11241
Peebles, P. J. E. 1993, Principles of Physical Cosmology (Princeton: Princeton Univ. Press)
Persson, C. M., et al. 2010, A&A, 515, A72
Pino, I., Martinazzo, R., & Tantardini, G. 2008, Phys. Chem. Chem. Phys., 10, 5545
Ramsbottom, C. A., Bell, K. L., & Berrington, K. A. 1994, J. Phys. B: At. Mol. Opt. Phys., 27, 2905
Schleicher, D. R. G., Galli, D., Palla, F., Camenzind, M., Klessen, R. S., Bartelmann, M., & Glover, S. C. O. 2008, A&A, 490, 521
Smith, M. S., Kawano, L. H., & Malaney, R. A. 1993, ApJS, 85, 219
Spergel, D. N., et al. 2007, ApJS, 170, 377
Stancil, P. C., Lepp, S., & Dalgarno, A. 1996, ApJ, 458, 401 (SLD96)
Stancil, P. C., & Zygelman, B. 1996, ApJ, 472, 102
Vernon, D. A., & Ferland, G. J. 1996, ApJS, 103, 467
Völk, H. J., R spasch, T., Winteler, C., Puy, D., Signore, M., & Dubrovich, V. 2009, A&A, 503, 47
Wagoner, R. V., Fowler, W. A., & Hoyle, F. 1967, ApJ, 148, 3
Wernli, M., Caruso, D., Bodo, E., & Gianturco, F. A. 2009, J. Phys. Chem. A., 113, 1121
Zaldarriaga, M., & Loeb, A. 2002, ApJ, 564, 52