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RATE OF FORMATION OF HYDROGEN MOLECULES BY THREE-BODY RECOMBINATION DURING PRIMORDIAL STAR FORMATION

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ABSTRACT

Astrophysical models of primordial star formation require rate constants for three-body recombination as input. The current status of these rates for H_2 due to collisions with H is far from satisfactory, with published rate constants showing orders of magnitude disagreement at the temperatures relevant for H_2 formation in primordial gas. This Letter presents an independent calculation of this recombination rate constant as a function of temperature. An analytic expression is provided for the rate constant which should be more reliable than ones currently being used in astrophysical models.

Key words: galaxies: formation – molecular processes – stars: formation

Online-only material: color figure

1. INTRODUCTION

A recent study (Turk et al. 2011) on the effects of varying the three-body recombination (TBR) rate of hydrogen during primordial star formation concluded that "the uncertainty in the three-body H_2 formation rate significantly limits our ability to model the density, temperature, and velocity structure of the gas close to the center of the collapse" and "the uncertainty in the outcome of collapse caused by our poor knowledge of the three-body H_2 formation rate coefficient cannot be so easily dealt with and represents a major limitation on our ability to accurately simulate the formation of the first stars in the universe" (Turk et al. 2011, p. 9, 10).

In this study, Turk et al. (2011) used three different published rate constants (Palla et al. 1983; Abel et al. 2002; Flower & Harris 2007) for the TBR process

$$\mathrm{H} + \mathrm{H} + \mathrm{H} \rightarrow \mathrm{H} + \mathrm{H}_2. \quad (1)$$

Two of these rate constants (Palla et al. 1983; Flower & Harris 2007) were based on the shock tube measurements of Jacobs et al. (1967) who gave analytic expressions for TBR and the inverse process of collision-induced dissociation (CID). The TBR rate adopted by Palla et al. (1983) was identical to the expression given by Jacobs et al. (1967) apart from a change in units. Flower & Harris (2007) used the CID expression given by Jacobs et al. (1967) together with their own determination of the equilibrium constant to derive a very different TBR rate constant. The discrepancy between these two TBR rate constants, therefore, is due to the adopted equilibrium constants that were used. The equilibrium constant used by Flower & Harris (2007) relies on the Saha equation and their determination of the H_2 partition function. When fitted to a simple temperature-dependent function, Flower & Harris (2007) found that their value is approximately 4.5 times greater than a similar fit obtained from the JANAF Thermochemical Tables at a temperature of 1000 K. Using this equilibrium constant together with the CID expression given in Jacobs et al. (1967) yielded a TBR rate constant which was approximately six times larger at $T = 1000$ K than the TBR expression given in Jacobs et al. (1967).

It appears that there are two separate reasons for the factors of 4.5 and 6 discrepancies at 1000 K. The first reason is fitting error. The experiments were performed in a temperature range of 2900–4700 K. When the same comparisons for the equilibrium constant and TBR rate are made in this experimental temperature range, both discrepancies are reduced to a factor of four over the whole range. In order to see this, the exact H_2 partition function must be used to compute the equilibrium constant, not the fitted value (Flower & Harris 2007) which is valid only for $T < 2000$ K. The second reason is the choice of atomic partition function which was assumed to be 2 for hydrogen in its $1s\ ^2S$ ground state (Flower & Harris 2007). This choice accounts for the nuclear spin degeneracy but not the electron spin degeneracy. Because the formation of H_2 occurs in the singlet electronic ground state, the electron spin degeneracy was assumed to be unity (D. R. Flower 2013, private communication). The present author disagrees with this assumption because three-fourths of the atomic collisions would still occur on the repulsive triplet electronic state even though they do not react. In order to account for only the one-fourth of collisions which can react, the atomic partition function used by Flower & Harris (2007) would need to be increased by a factor of two which would reduce their equilibrium constant by a factor of four. Therefore, the TBR rate of Flower & Harris (2007) would also need to be reduced by this same factor of four. This would, upon use of the exact H_2 partition function, bring their TBR rate into excellent agreement with the rate of Jacobs et al. (1967) and Palla et al. (1983) at temperatures in the experimental range.

While this resolves the discrepancy between two of the three rate constants used in the Turk et al. (2011) study, it does not imply that the rate constants are reliable. The experimental paper (Jacobs et al. 1967) upon which these TBR rate constants are based cautions that their data lies in the middle of a range of other experimental data whose values vary over an order magnitude. Furthermore, substantial errors may be introduced by extrapolating collisional data, obtained over a small range of temperatures, to temperatures that lie outside that range. All three of the TBR rates considered in the Turk et al. (2011) study are based on extrapolations for temperatures between 300 and 2900 K. The third and smallest TBR rate (Abel et al. 2002) uses an extrapolation of classical trajectory calculations (Orel 1987) which were performed at temperatures below 300 K. This extrapolation assumes an inverse temperature dependence which resembles that of the experiment (Jacobs et al. 1967)

and consequently has a sudden change in slope at 300 K. It is desirable, therefore, to perform an independent calculation which does not rely on extrapolations and is reliable over the temperature range required by the astrophysical models.

2. CALCULATIONS

In this Letter, we report results of quantum mechanical calculations of TBR rate constants for the collision of three hydrogen atoms in the temperature range $300 < T < 10{,}000$ K. We use a Sturmian representation which provides a quadrature of the two-body continuum and may be used to generate a complete set of states within any desired TBR pathway (Forrey 2013). The effective TBR and CID rate constants at local thermodynamic equilibrium (LTE) may then be defined by

$$k_r \equiv \sum_{b,u} k_{u\to b} \frac{g_u \exp(-E_u/k_B T)}{Q_H^2 Q_T} \tag{2}$$

$$k_d \equiv \sum_{b,u} k_{b\to u} \frac{g_b \exp(-E_b/k_B T)}{Q_{\mathrm{H}_2}}, \tag{3}$$

where b designates a bound state with energy E_b and u designates an unbound state with energy E_u. These states are defined by their associated vibrational and rotational quantum numbers v and j, and the zero of potential energy for both E_b and E_u is assumed to be at infinite separation. The statistical factors are given by $g = (2j+1)(2I+1)$ with the nuclear spin $I = 0$ for para-H_2 and $I = 1$ for ortho-H_2. With this definition for g, the atomic partition function is $Q_{\mathrm{H}} = 4$ as described above. The molecular partition function Q_{H_2} and the translational partition function Q_T are defined by

$$Q_{\mathrm{H}_2} = \sum_b g_b \exp(-E_b/k_B T) \tag{4}$$

$$Q_T = \frac{(\pi m k_B T)^{3/2}}{h^3}, \tag{5}$$

where h is Planck's constant, k_B is Boltzmann's constant, T is the temperature, and m is the mass of H. Detailed balance of the rate coefficients $k_{b\to u}$ and $k_{u\to b}$ may be used to show that the above definitions yield the statistical Saha equation

$$\frac{k_r}{k_d} = \frac{[\mathrm{H}_2]}{[\mathrm{H}]^2} = \frac{Q_{\mathrm{H}_2}}{Q_{\mathrm{H}}^2 Q_T} \tag{6}$$

for the thermalization of the continuum. For the results reported here, we assume that the system is in equilibrium. Corrections for non-LTE conditions are estimated to be small. The calculations use an energy sudden approximation which was tested for He+H+H by comparing with coupled states calculations (Forrey 2013). Results from the two methods showed good agreement at temperatures greater than 600 K. The calculations also assume that the atoms are distinguishable which should be a good approximation at the high temperatures under consideration and is consistent with classical calculations. The BKMP2 (Boothroyd et al. 2002) potential energy surface (PES) was employed for the calculations. Previous quasiclassical calculations (Esposito & Capitelli 2009) found that the BKMP2 PES gave very similar results compared to the LSTH PES (Truhlar & Horowitz 1979) over the same temperature range considered in the present work.

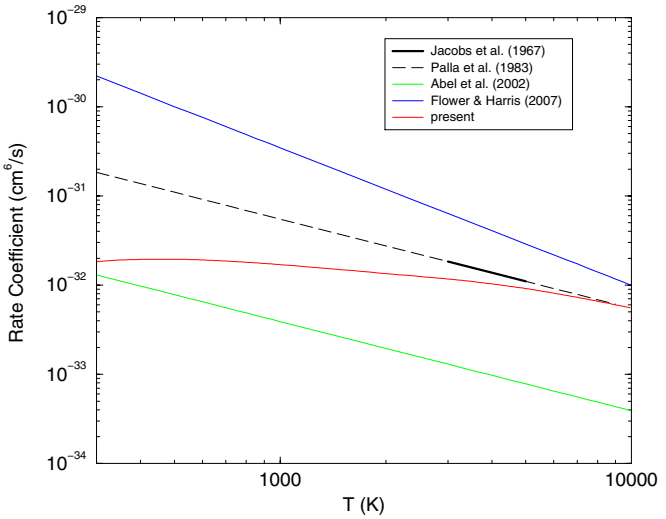

Figure 1. TBR rate constant for H+H+H. The present results show a much flatter temperature dependence than any of the rates used in the gravitational collapse simulations (Turk et al. 2011).

(A color version of this figure is available in the online journal.)

3. RESULTS

Figure 1 shows the results of the present calculations together with the three TBR rate constants considered in the study of Turk et al. (2011). The present results are smaller than those of Flower & Harris (2007) and Palla et al. (1983) over the entire temperature range shown. These curves are both based on the experimental data of Jacobs et al. (1967) as discussed above. Compared to the Palla et al. (1983) curve, we find good agreement with the extrapolation at high temperatures but poor agreement at low temperatures. We see the opposite effect when compared to the Abel et al. (2002) curve. The present calculations produce a much flatter temperature dependence than the other three curves. This flat temperature dependence is in good agreement with quasiclassical results (Esposito & Capitelli 2009) which were also computed using the BKMP2 PES. The magnitude of the present results agree with those of Esposito & Capitelli (2009) to within a factor of two over the entire temperature range shown. They also agree to within a factor of two with Jacobs et al. (1967) and Orel (1987). Therefore, the factor of $\sim$100 uncertainty which was introduced by the various extrapolations is estimated to be reduced to a factor of $\sim$2 when the present results are used.

4. CONCLUSIONS

The results of the present calculations may be conveniently expressed by the function

$$k_r = 6\times 10^{-32} T^{-1/4} + 2\times 10^{-31} T^{-1/2} \tag{7}$$

using the same units as in Figure 1. This expression is virtually identical to the calculations for $T = 600$–6000 K and not too different at the endpoints of the range shown in the figure. This analytic function should be reliable for temperatures required by the hydrodynamics simulations. Based on previous simulations (Turk et al. 2011), it is expected that the gravitational collapse will produce a gas distribution which is somewhere in between the spherical distribution obtained using the Abel et al. (2002) rate constant and the bar-shaped distribution obtained using the Palla et al. (1983) rate constant.

It is noteworthy that recent numerical simulations of gravitational fragmentation (Clark et al. 2011) adopted a TBR rate constant which was in between that of Palla et al. (1983) and Abel et al. (2002). This rate constant was due to Glover (2008) who used the CID rate constants of Martin et al. (1996) together with the fitted equilibrium constant of Flower & Harris (2007) which as noted above is four times too large when $T < 2000$ K. It is recommended that future astrophysical simulations of gravitational collapse employ the revised equilibrium and TBR rate constants accordingly.

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