

1-1-2004

## Cooling due to collisions between hydrogen molecules and helium atoms

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COOLING DUE TO COLLISIONS BETWEEN HYDROGEN  
MOLECULES AND HELIUM ATOMS

by

Lisa Ann Grew

Bachelor of Arts, Physics  
Boston University  
2001

A thesis submitted in partial fulfillment  
of the requirements for the

**Master of Science Degree in Physics**  
**Department of Physics**  
**College of Sciences**

**Graduate College**  
**University of Nevada, Las Vegas**  
**December 2004**

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Cooling Due to Collisions Between Hydrogen Molecules and

Helium Atoms

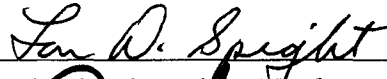
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## ABSTRACT

### **Cooling Due to Collisions Between Hydrogen Molecules and Helium Atoms**

by

Lisa Ann Grew

Dr. Stephen Lepp, Examination Committee Chair  
Professor of Physics  
University of Nevada, Las Vegas

This study concerns the cooling that occurs in molecular clouds. The contribution to the cooling in these clouds by collisions between hydrogen molecules and helium atoms was investigated. The semi-classical method was used to calculate the rate coefficients for all He-induced H<sub>2</sub> ro-vibrational transitions, and these were compared with previous quantum mechanical calculations. The steady state ro-vibrational level populations were found and used to compute the cooling function over a range of temperatures and densities. The time required to reach steady state is discussed, and a comparison is made of the results to corresponding values in thermodynamic equilibrium. The cooling function is compared to a previous quantum mechanical calculation. The suitability of the semi-classical method is discussed.

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## ACKNOWLEDGMENTS

I thank Dr. Lepp for his patience and support while I completed this project. I also thank the members of my examination committee for their time. This work was supported by National Science Foundation Grant AST0087348.

I thank Mom and Dad most of all; everything I have accomplished was made possible by you.



## CHAPTER 1

### INTRODUCTION

The mean particle density of the interstellar medium is  $1 \text{ cm}^{-3}$ . It is composed of mostly hydrogen; helium accounts for approximately 10% of the gas. The interstellar medium is not smooth, but clumped. There are partly ionized regions with densities of  $0.1 \text{ cm}^{-3}$  and temperatures of  $10^4 \text{ K}$ ; there are neutral clouds with densities of  $10\text{-}10^3 \text{ cm}^{-3}$  and low temperatures of about  $100 \text{ K}$ ; and in between the dense regions there are completely ionized regions with density  $10^2 \text{ cm}^{-3}$  and temperatures of  $10^6 \text{ K}$ .

Molecular clouds are more dense than these regions (about  $10^3\text{-}10^4 \text{ cm}^{-3}$ ) and very cool, with temperatures as low as  $10 \text{ K}$ . Since few or no 21-cm lines are observed it appears that most of the hydrogen is in molecular form (Dyson & Williams 1997).

This study concerns the cooling that occurs in molecular clouds with temperatures much higher than  $10 \text{ K}$ , sometimes attained when the clouds are heated by shocks. Observations of the molecular cloud in Orion show that shock heating occurs there. Shock heating is believed to be quite common in molecular clouds. The extremely high temperatures reached in some shock-heated clouds could cause the dissociation of molecular hydrogen or its vibrational excitation; it is possible that magnetic fields could mitigate this effect by limiting the temperature (Flower 1990).

Collisions between helium atoms and hydrogen molecules contribute to cooling

in these shocked regions, as well as in the early universe. The ro-vibrational levels of  $\text{H}_2$  can be populated in many ways besides by collisions with helium. Collisions with hydrogen atoms and other hydrogen molecules occur, as does UV and X-ray pumping (Balakrishnan *et al.* 1999b). In the interstellar molecular clouds, besides with itself  $\text{H}_2$  is most likely to collide with helium. This work studies cooling due to the collisional excitation of hydrogen molecules by helium atoms.

Understanding the interaction between He and  $\text{H}_2$  is important for interpreting observed  $\text{H}_2$  spectra. The Infrared Space Observatory, among others, has observed many  $\text{H}_2$  emission lines. These can yield information about the physical state of the cloud. When molecular spectra come from regions that are not in thermal equilibrium, to interpret them it is necessary to know about the processes, including collisions, which govern the ro-vibrational level populations. The rate coefficients describing collisions can be used to calculate the intensities of  $\text{H}_2$  transitions to compare with observations.

Collisions between He and  $\text{H}_2$  have been investigated in many studies. Rate coefficients were calculated by Flower *et al.* (1998) and Balakrishnan *et al.* (1999a, 1999b), and the cooling due to excitation by He was calculated by Le Bourlot *et al.* (1999). The quantum mechanical calculation of Flower *et al.* (1998) used the coupled-channels method, with the He- $\text{H}_2$  potential of Muchnick & Russek (1994) and the harmonic oscillator wavefunctions in scattering calculations. Rate coefficients were presented for  $100 \leq T \leq 6000$  K up to vibrational level  $\nu = 3$ , with  $j \leq 8$ . The quantum mechanical calculation of Balakrishnan *et al.* (1999a, 1999b) was similar but used the exact vibrational wavefunctions in the scattering calculations; rate coefficients were

presented for  $10 \leq T \leq 5000$  K up to  $v = 1$  and low  $j$ , and  $100 \leq T \leq 4000$  K up to  $v = 6$ , with  $j \leq 11$ . Le Bourlot *et al.* (1999) presented the cooling function due to collisions with H, H<sub>2</sub>, and He, using the rate coefficients computed in Flower *et al.* (1998) in the He-H<sub>2</sub> cooling calculation. The cooling function was given for  $100 \leq T \leq 10,000$  K with densities ranging from 1 to  $10^8$  cm<sup>-3</sup>.

This study uses the semi-classical method to calculate the rate coefficients for all helium-induced H<sub>2</sub> ro-vibrational transitions. The steady state level populations were found and used to compute the cooling function for  $500 \leq T \leq 20,000$  K and  $1 \leq n_{\text{H}} \leq 10^8$  cm<sup>-3</sup>. The time required to reach steady state is discussed, and a comparison of the results to corresponding values in thermodynamic equilibrium is made. The cooling function is compared to that presented in Le Bourlot *et al.* (1999) at a low density.

## CHAPTER 2

### METHODOLOGY

Rate coefficients for all H<sub>2</sub> ro-vibrational transitions induced by collisions with helium atoms were calculated using cross section data provided by S. Lepp. Steady state level populations of H<sub>2</sub> were determined and used to calculate cooling rates for a range of physical conditions.

#### Calculation of Rate Coefficients

The data provided by S. Lepp were used to calculate cross sections at constant energy for all collisionally-induced H<sub>2</sub> transitions. The data set was generated by applying the semi-classical method employed in Lepp *et al.* (1995) to the He-H<sub>2</sub> system (Balakrishnan *et al.* 1999b). Standard classical trajectories were used and the classical equations of motion were solved. The calculations used the H<sub>2</sub> potential of Schwenke (1998) and the He-H<sub>2</sub> interaction potential of Muchnick & Russek (1994). The data was generated for a range of temperatures,  $500 \leq T \leq 30,000$  K, and averaged over 10,000 trajectories.

The cross section for a transition from ro-vibrational state  $l$  to state  $m$  at constant energy  $E$  is given by

$$\sigma_{lm}(E) = \pi b_{max}^2 \frac{n_{lm}}{10,000};$$

$b_{max}$  is the maximum impact parameter and  $n_{lm}$  is the number of trajectories for which the molecule's initial state is  $l$  and final state is  $m$ . The error associated with each cross section is given by

$$\delta \sigma_{lm}(E) = \pi b_{max}^2 \frac{\sqrt{n_{lm}}}{10,000}.$$

To compute the rate coefficient for a transition, the corresponding cross section must be averaged over a Boltzmann distribution. The rate coefficient  $k$  for a given transition  $l \rightarrow m$  is

$$k_{lm}(T) = v_{th} \bar{\sigma}_{lm}(T),$$

where  $v_{th}$  is the thermal velocity of the incoming He atom at temperature  $T$ . The average cross section for a transition  $l \rightarrow m$  is given by

$$\bar{\sigma}_{lm}(T) = \frac{\int_0^{\infty} E \sigma_{lm}(E) e^{-E/k_B T} dE}{\int_0^{\infty} E e^{-E/k_B T} dE},$$

where  $k_B$  is Boltzmann's constant. Defining as  $T_E$  the temperature associated with energy  $E$ , as in  $E = k_B T_E$ , this can be rewritten as

$$\bar{\sigma}_{lm}(T) = \frac{\int_0^{\infty} T_E \sigma_{lm}(T_E) e^{-T_E/T} dT_E}{\int_0^{\infty} T_E e^{-T_E/T} dT_E}.$$

The integral in the denominator evaluates to  $1/T^2$ .

The integration was performed using the trapezoid method. Cross sections were available at seven temperatures from 500 K to 30,000 K; at higher temperatures, they were represented by their value at 30,000 K. The integral rewritten as a sum is:

$$\bar{\sigma}_{lm}(T) = \frac{1}{T^2} \sum_{n=1}^7 T_n \sigma_{lm}(T_n) e^{-T_n/T} \Delta T_n,$$

with  $\Delta T_n = T_n - T_{n-1}$ . It was assumed that the cross section is zero at  $T = 0$  K, so that  $\Delta T_1 = 1/2 T_1$ .

This procedure was used to find all de-excitation rates. The method used to compute the cross section points allowed for the possibility that an upward transition could occur in a collision with insufficient energy transfer. To avoid the inaccuracy caused by those instances, the corresponding excitation rates were found by detailed balance:

$$k_{lm}(T) = \frac{g_m}{g_l} k_{ml} e^{-E_m/k_B T};$$

$$E_{lm} = E_m - E_l.$$

Here,  $g_m$  is the statistical weight of level  $m$ .

### Solving for the Steady State Level Populations

Once all of the rate coefficients were calculated, they were used, along with the Einstein coefficients for spontaneous transitions (Turner *et al.* 1977), to solve for the steady state ro-vibrational level populations of the H<sub>2</sub> molecules.

The population of a given  $(\nu, j)$  level can be affected by several processes: collisional excitation, collisional de-excitation, and spontaneous transition into or out of the level. Other processes, including reactive processes that convert between ortho-H<sub>2</sub> and para-H<sub>2</sub>, were not considered in this study. The equation governing a particular level  $l$  is (Spitzer 1978)

$$\frac{dn_l}{dt} = -n_l \sum_m n_{\text{He}} k_{lm} - n_l \sum_{m < l} A_{lm} + \sum_m n_m n_{\text{He}} k_{ml} + \sum_{m > l} n_m A_{ml}.$$

This equation was modified and put into a simple matrix form,

$$\frac{dN}{dt} = MN,$$

where M is a 301 x 301 matrix containing all  $n_{\text{He}}k$  and A terms and N is a 301 x 1 matrix holding the fractional populations of each of the 301  $(\nu, j)$  levels considered in this study. The density of helium atoms was set at  $n_{\text{He}} = 0.10 n_{\text{H}}$ . The initial condition used at time  $t = 0$  s of the ortho- and para-H<sub>2</sub> ground states was  $N(0,0) = N(0,1) = 0.5$ . This equation was solved for the steady state level populations, or 'stepped forward in time' until  $dN/dt = 0$ . This procedure was completed for a large range of densities,  $1 \leq n_{\text{H}} \leq 10^8 \text{ cm}^{-3}$ , and temperatures,  $500 \leq T \leq 30,000 \text{ K}$ .

## Calculating the Cooling Rates

The steady state populations  $n_l$  were used in computing  $\Lambda(\text{H}_2)$ , the cooling rate per  $\text{H}_2$  molecule:

$$\Lambda(\text{H}_2) = \sum_{l,m} (E_l - E_m) n_l A_{lm} \text{ erg/s} ,$$

$$E_l > E_m .$$

Once the level populations have reached steady state, the  $\text{H}_2$  molecules can lose energy from photons emitted in spontaneous downward transitions. It is assumed that the gas is optically thin at the photonic wavelengths so that the photons escape the cloud, resulting in cooling. This assumption is less reliable for the higher density clouds, where photons are more likely to be reabsorbed before escaping.

## Analytic Fit to Rate Coefficients

The de-excitation rate coefficients were fitted to an analytic form adopted in Le Bourlot *et al.* (1999):

$$\log k_{v_j, v' j'}(T) = a + \frac{b}{t} + \frac{c}{t^2} .$$

The rate coefficient  $k_{v_j, v' j'}(T)$  is in units of  $\text{cm}^3/\text{s}$  and  $t = (T(\text{K}))/1000 + dt$ ;  $dt$  is a constant adjusted to make sure the rate coefficients don't diverge at low temperatures. The value of  $dt$  used was 1.471. This fit was performed for seven temperatures in the range  $1000 \leq T \leq 30,000$  K. Approximately 13,000 rate coefficients were included.

To determine the goodness of the fit,  $\chi^2$  values were calculated. The form used was



$$\chi^2 = \sum_{i=1}^6 \{ [y_i - y_{fit}(T_i)] / \sigma_i \}^2,$$

where  $y_i$  is the logarithm of the calculated rate coefficient at the  $i^{\text{th}}$  temperature,  $y_{fit}$  is the analytic form presented above, and the weight factor  $\sigma_i = 3$  for the two lowest temperatures and  $\sigma_i = 1$  otherwise. Figure 1 shows the  $\log \chi^2$  values for each transition.

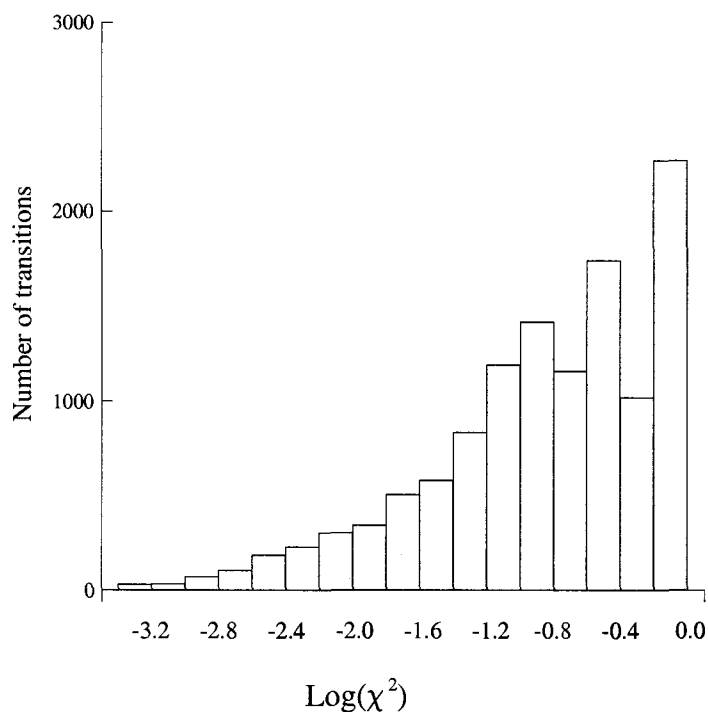


Figure 1. Values of  $\log(\chi^2)$  from the analytic fit to de-excitation rate coefficients.

Samples of the fits to the calculated rate coefficients are presented below. Figure 2 shows the fit to a pure rotational transition, and a ro-vibrational transition is shown in Figure 3.

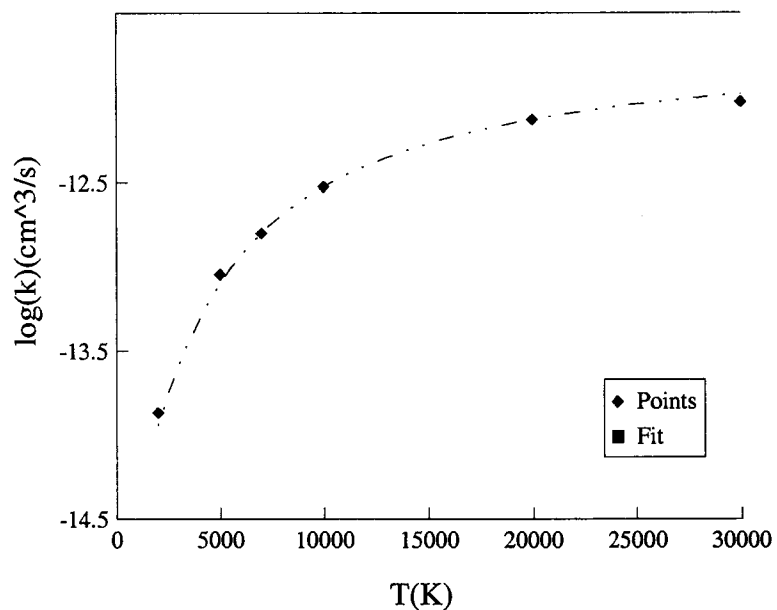


Figure 2. Fit to the calculated rate coefficients for the rotational transition (2,10) to (2,0).

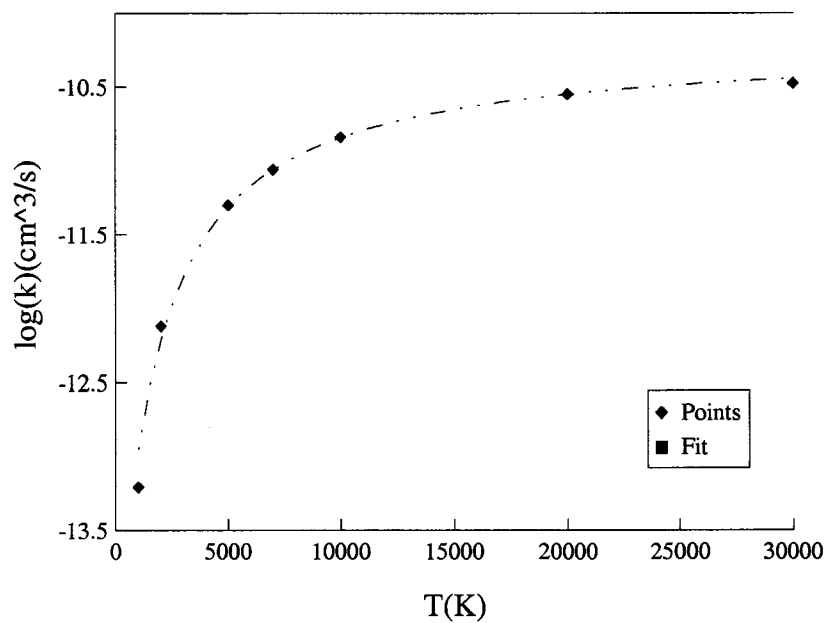


Figure 3. Fit to the calculated rate coefficients for the ro-vibrational transition (1,6) to (0,8).

## CHAPTER 3

### CALCULATION RESULTS AND ANALYSIS

#### Presentation of Cross Sections

Selected semi-classical and quantum mechanical cross sections for collisions between He and H<sub>2</sub> are presented in Figure 4 (adapted from Balakrishnan *et al.* 1999b). Within each plot, the error bars for each semi-classical cross section at the lowest temperature shown are the size of the symbol; those for cross sections at higher temperatures are smaller than the symbol. The semi-classical cross sections are larger than the quantum mechanical cross sections at higher temperatures, and drop to zero sharply at low temperatures. It is apparent that the semi-classical calculation provides good results for rotational transitions at temperatures above 6000 K. A comparison between the semi-classical and quantum mechanical cross sections for ro-vibrational transitions shows that the semi-classical calculation will give good results at temperatures above 10,000 K.

#### Analysis of Rate Coefficients

Rate coefficients for ro-vibrational transitions in H<sub>2</sub> due to collisions with helium atoms were calculated in this work with the semi-classical trajectory treatment of

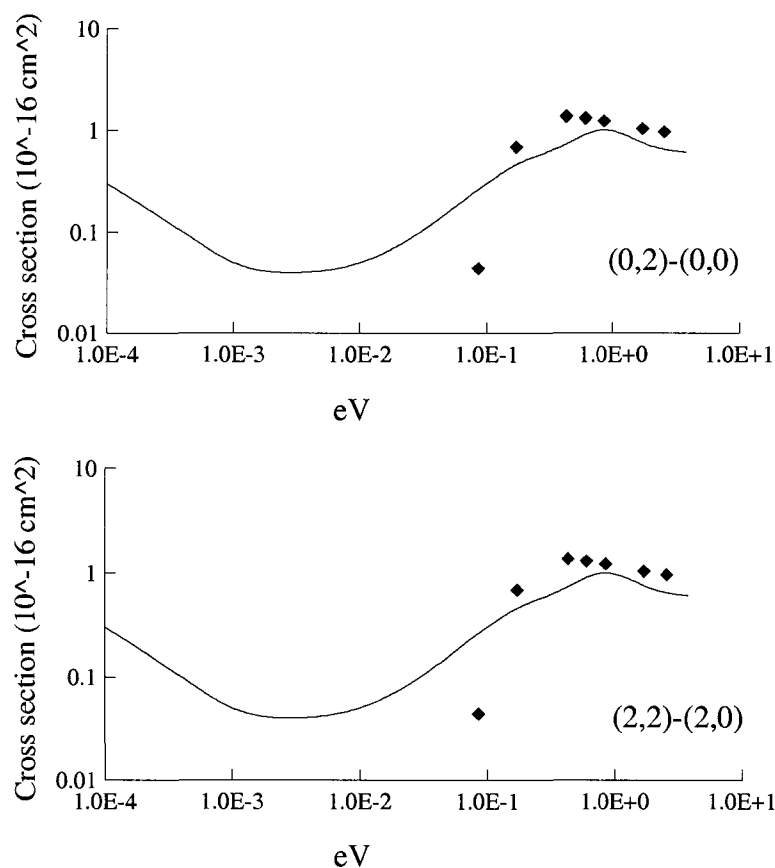


Figure 4. Quantum mechanical cross sections (solid line) from Balakrishnan *et al.* (1999b) and semi-classical cross sections (solid symbols) from this work for selected rotational transitions.. The error bars for each cross section at the lowest temperature shown are the size of the symbol; those for cross sections at higher temperatures are smaller than the symbol.

He-H<sub>2</sub> collisions described above. The simulations used the Schwenke (1998) H<sub>2</sub> potential and the Muchnick & Russek (1994) He-H<sub>2</sub> potential energy surface (Balakrishnan *et al.* 1999b). These rate coefficients were compared to those calculated by Flower *et al.* (1998). That quantum mechanical calculation used a harmonic oscillator H<sub>2</sub> potential for vibrational wavefunction calculations and the same He-H<sub>2</sub> potential energy surface as this study. The rate coefficients of this work were also compared to those presented in Balakrishnan *et al.* (1999a, 1999b). That study used

the same potentials, the exact vibrational wavefunctions, and did a full quantum mechanical calculation.

In this study, rate coefficients were calculated for transitions involving vibrational levels  $v \leq 14$  and rotational levels  $j \leq 31$  in the temperature range  $500 \leq T \leq 30,000$  K. They were compared to the rate coefficients calculated in Flower *et al.* (1998) presented at [http://ccp7.dur.ac.uk/cooling\\_by\\_h2/index.html](http://ccp7.dur.ac.uk/cooling_by_h2/index.html). These rate coefficients are for transitions involving vibrational levels  $v \leq 3$  and rotational levels  $j \leq 16$  in the temperature range  $100 \leq T \leq 6000$ K. The rate coefficients calculated in this work were also compared to rate coefficients presented in Balakrishnan *et al.* (1999a, 1999b), which are for transitions involving  $v \leq 6$  and  $j \leq 11$  in the temperature range  $10 \leq T \leq 5000$  K.

#### Comparison to Flower *et al.* (1998)

A direct comparison was made at  $T = 2000$  K of de-excitation rate coefficients from the present work with all those published in Flower *et al.* (1998). Of 601 total de-excitation rate coefficients, the majority (536) of those in the present study are higher than those of Flower *et al.* (1998). Of those that are lower, most involve transitions for which  $\Delta v = -1$  and  $\Delta j = 0, 2, \text{ or } 4$ .

Several plots of rate coefficients from this work and that of Flower *et al.* (1998) for representative pure vibrational, pure rotational, and mixed transitions are presented below. The vertical axes of every plot cover the same range in order to facilitate comparison.

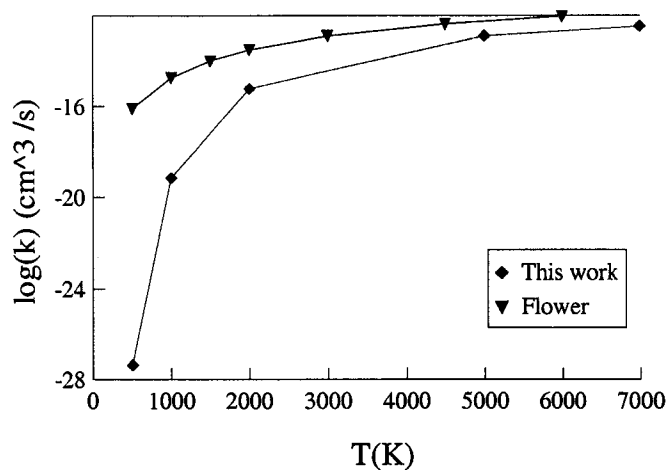


Figure 5. Pure vibrational transition (1,5) to (0,5).

A low-lying pure vibrational transition is shown in Figure 5. This transition is one of the minority for which the semi-classical rate coefficients are lower than those of Flower *et al.* (1998). There is severe disagreement at lower temperatures; the rate coefficients of this work often do not approach those of Flower *et al.* (1998) until

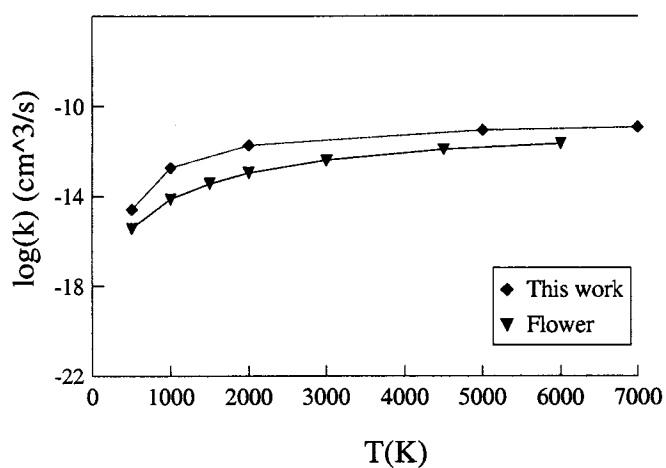


Figure 6. Pure vibrational transition (2,6) to (1,6).

temperatures of several thousand degrees. This trend is also seen in the  $\Delta v = -1$  pure vibrational transitions (1,2) to (0,2), (1,3) to (0,3), and (1,4) to (0,4), but not for those originating in levels with  $v = 1, j > 5$ .

Two pure vibrational transitions from slightly higher levels are represented in Figures 6 and 7. Following the general trend, agreement improves with increasing temperature.

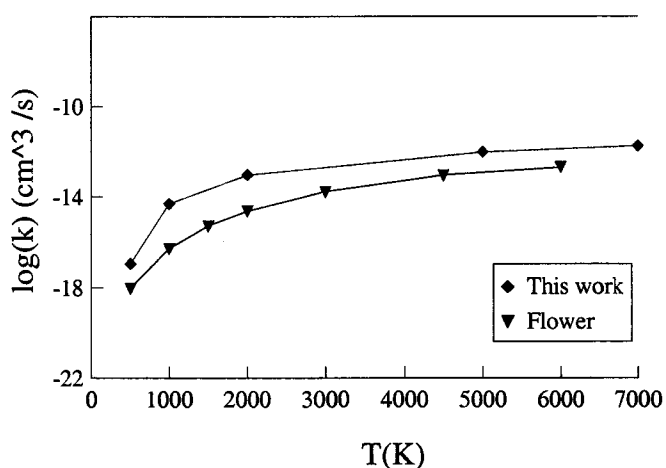


Figure 7. Pure vibrational transition (3,7) to (1,7).

Several pure rotational transitions are shown for  $|\Delta j| = 2, 4, 6,$  and  $8$  in Figures 8 through 12. The largest disagreements for transitions are generally found at  $T = 500$  K; as temperature increases, the discrepancies decrease. Rate coefficients from the present study are higher than those of Flower *et al.* (1998) in all cases shown. At higher temperatures ( $T > 2000$  K) agreement ranges from within a few percent to about 15%.

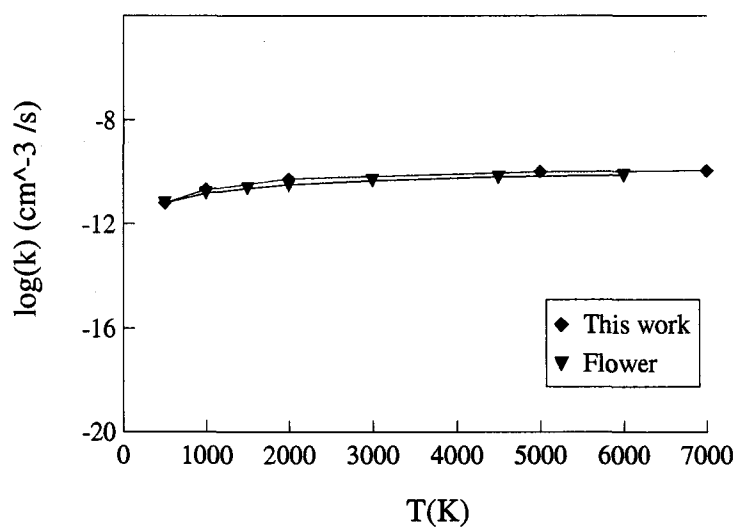


Figure 8. Pure rotational transition (0,2) to (0,0).

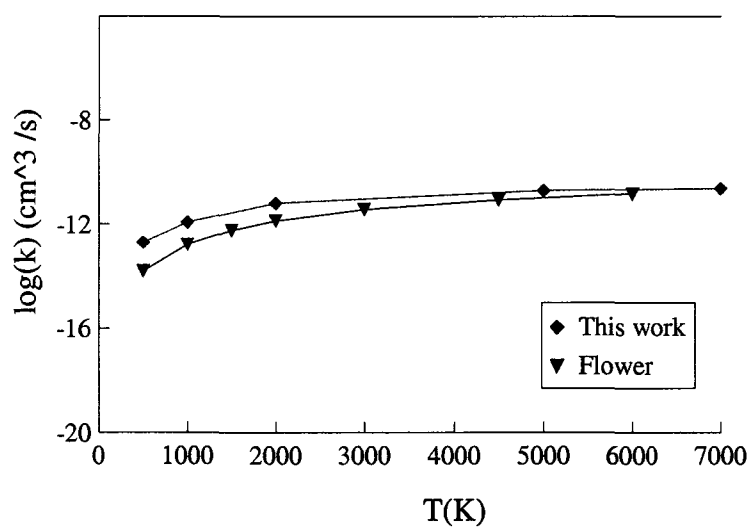


Figure 9. Pure rotational transition (1,7) to (1,3).



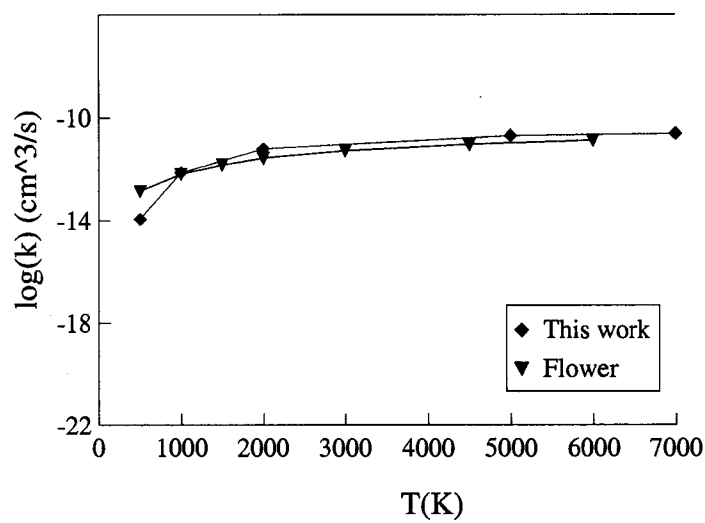


Figure 10. Pure rotational transition (2,4) to (2,0).

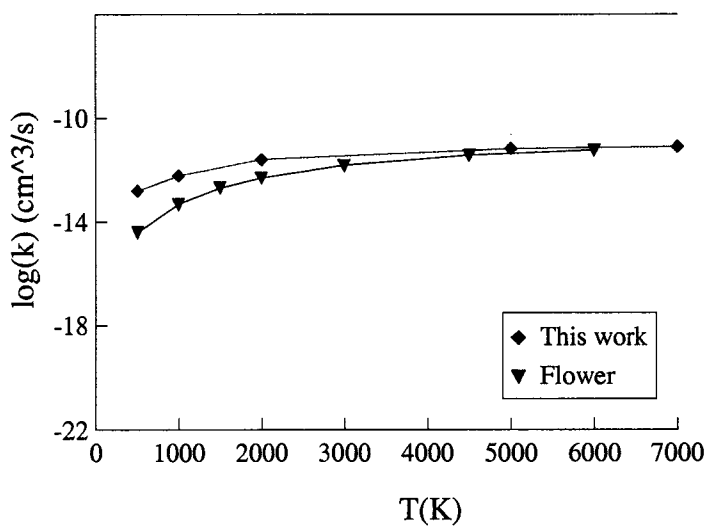


Figure 11. Pure rotational transition (3,7) to (3,1).

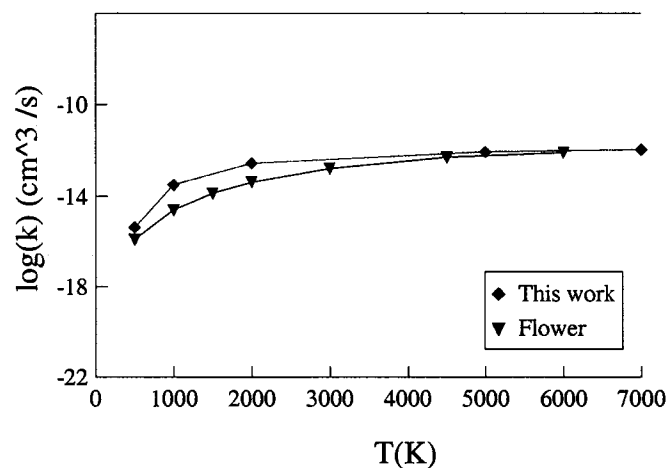


Figure 12. Pure rotational transition (3,8) to (3,0).

An example of a low-lying ro-vibrational transition is shown in Figure 13. The agreement at  $T = 500$  K is unusually good.

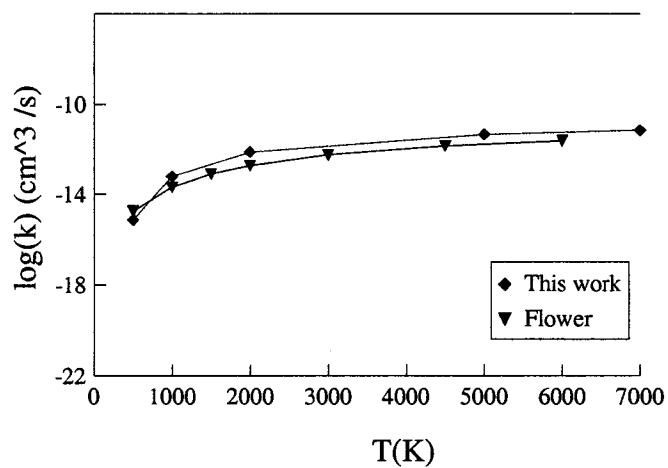


Figure 13. Ro-vibrational transition (1,6) to (0,8).

The comparison of all rate coefficients at  $T = 2000$  K illuminated those for which

discrepancies between this work and Flower *et al.* (1998) are highest. All of these rate coefficients differ by over three orders of magnitude, and all represent transitions to or from a rotational level higher than  $j = 6$ . The various energies of each transition differ by as much as a factor of ten and are not abnormally high or low; the average energy corresponds to  $T \approx 3500\text{K}$ . These were transitions with  $\Delta v = \pm 1, 2, \text{ and } 3$  and  $\Delta j = \pm 6, 8, 10, \text{ and } 12$ .

This comparison also revealed those rate coefficients with the best agreement (within 10% or less) at  $T = 2000\text{ K}$ . These represent ro-vibrational transitions with  $\Delta v = 0$  or  $-1$  and  $\Delta j = -2, 6, \text{ or } 8$ . The average energy of these transitions corresponds to  $T \approx 800\text{ K}$ .

Analysis of the two sets of rate coefficients shows that the majority of rate coefficients calculated in this work are higher than those calculated in Flower *et al.* (1998), and that agreement ranges from a few percent to several orders of magnitude (at low temperatures). Rate coefficients from the present work for low-lying pure vibrational transitions from levels  $v = 1, j \leq 5$  at low temperatures are evidently quite unreliable. In general rate coefficients for pure rotational transitions calculated in this work agree well with those of Flower *et al.* (1998). The worst agreement comes from transitions originating in rotational levels  $j \geq 8$  with average transitional energies of corresponding temperature  $T \approx 3500\text{ K}$ . The best agreement comes from transitions between some closely spaced ( $T \approx 800\text{ K}$ ) levels. In all cases, agreement between rate coefficients calculated in this work and that of Flower *et al.* (1998) increases with increasing temperature.

Comparison to Balakrishnan *et al.* (1999a, 1999b)

In Balakrishnan *et al.* (1999b) a comparison was carried out of the quasi-classical trajectory method to the full quantum mechanical method of calculating cross sections for He-H<sub>2</sub> collisions. It was concluded that the quasi-classical trajectory method is only dependable for energies above 0.5 eV for pure rotational transitions and above 1 eV for ro-vibrational transitions. A comparison of the rate coefficients from this work with those of Balakrishnan *et al.* (1999b) agrees with this conclusion.

A representative pure rotational transition is depicted in Figure 14. It is clearly seen that agreement between quasi-classical and quantum mechanical calculations is better at high temperatures.

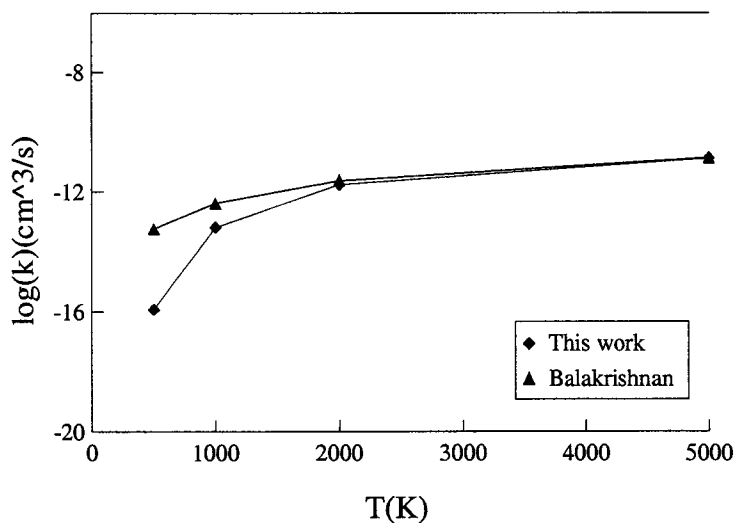


Figure 14. Rotational transition (0,5) to (0,1).

A comparison of several rate coefficients at  $T = 2000$  K for pure rotational transitions from this work and that of Balakrishnan *et al.* (1999b) is shown in Table 1. Even for transitions within the higher vibrational levels, agreement is within a factor of 1.5.

Table 1. Rate coefficients (in units of  $\text{cm}^3/\text{s}$ ) for pure rotational transitions at  $T = 2000$  K.

$v_j, v_j'$	This work	Balakrishnan
22,20	6.97E-11	4.69E-11
24,20	6.16E-12	4.83E-12
24,22	5.88E-11	4.96E-11
32,30	7.69E-11	5.35E-11
34,30	8.07E-12	6.64E-12
34,32	7.15E-11	6.05E-11
44,40	9.66E-12	8.63E-12
44,42	8.31E-11	7.21E-11
46,44	6.80E-11	4.63E-11
54,50	1.22E-11	1.08E-11
54,52	9.85E-11	8.44E-11
56,52	1.67E-11	1.34E-11
64,60	1.51E-11	1.31E-11
64,62	1.12E-10	9.73E-11
66,62	2.09E-11	1.77E-11

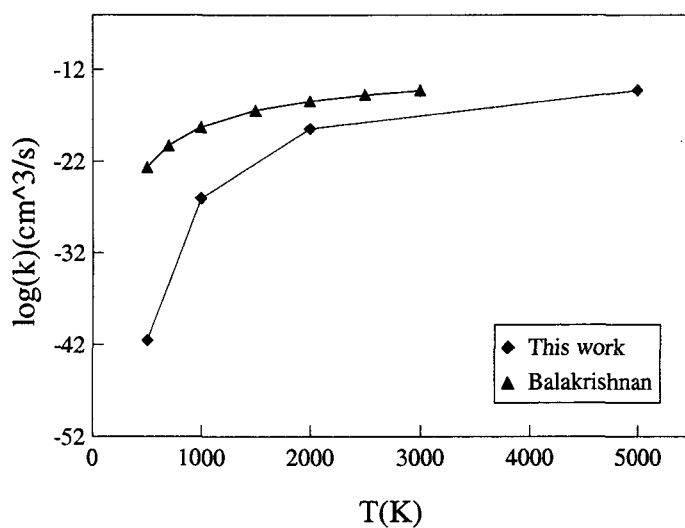


Figure 15. Ro-vibrational transition (0,1) to (1,3).

In Figure 15, rate coefficients for a representative ro-vibrational transition are shown. Agreement between the two calculations is poor, but shows signs of improving at high temperatures.

The rate coefficients calculated in this work appear to support the conclusion of Balakrishnan *et al.* (1999b) that the quasi-classical calculations, especially those for ro-vibrational transitions, are unreliable at low temperatures.

### Time to Equilibrium

The timescale for the H<sub>2</sub> level populations to come to equilibrium depends on the temperature and density of the cloud, as well as the initial level distribution. Once the steady state populations were determined, the cooling function was evaluated. Steady state is attained when  $dn_{v,j}/dt = 0$ ; that is, when the level populations are redistributed from their initial values (half in level (0,0) and half in level (0,1)) to all levels.

In low density, low temperature models, the time to equilibrium was on the order of thousands of years. In high density, high temperature models the timescale was much shorter at one year or less. One representative system is presented in Figure 16, which shows how the fractional populations of the (0,0) and (0,1) levels change with time. At  $T = 1000$  K,  $n_{\text{H}} = 10^4$  cm<sup>-3</sup>, the timescale to equilibrium is about ten years.

### H<sub>2</sub> Steady State Level Populations

The extent to which the higher ro-vibrational levels are populated in steady state was investigated. For  $T < 2000$  K and  $n_{\text{H}} < 100$  cm<sup>-3</sup>, there is not significant population above the lowest 10 or so levels. Thus the cooling associated with these clouds comes

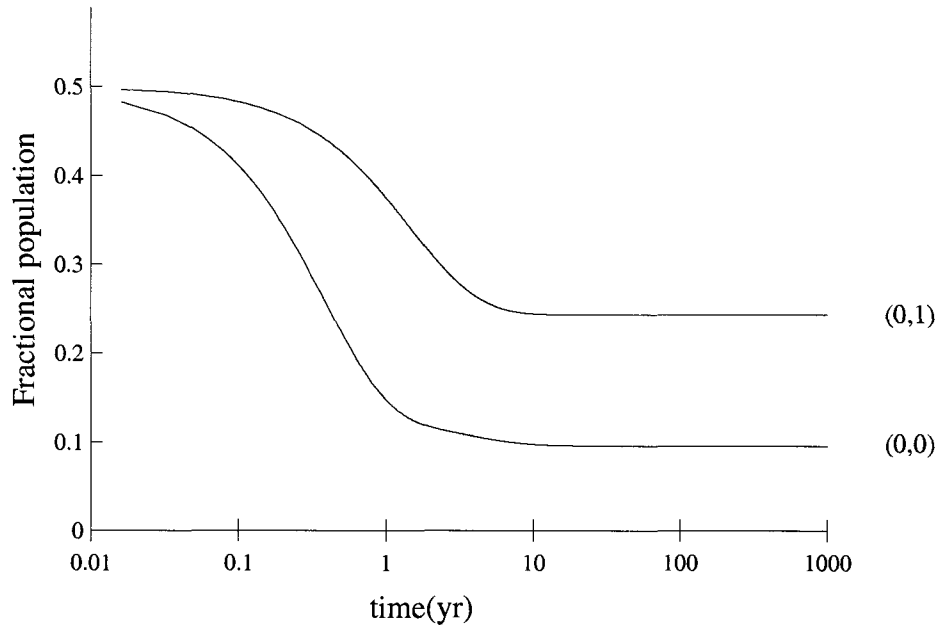


Figure 16. Time to equilibrium for levels (0,0) and (0,1) at  $T = 1000$  K,  $n_H = 10^4$  cm<sup>-3</sup>.

primarily from rotational transitions within the  $v = 0$  manifold. As temperature and density increase, so do the populations of higher ro-vibrational levels. Not until  $T > 5000$  K and  $n_H > 10^7$  cm<sup>-3</sup> is it likely that the highest levels will be populated.

### Steady State Populations Compared With Local Thermodynamic Equilibrium

A comparison was made of the steady state populations obtained and those that would occur in local thermodynamic equilibrium (LTE) as described by the Boltzmann distribution:

$$\frac{n_2}{n_1} = \frac{g_2}{g_1} e^{-\frac{(E_2 - E_1)}{k_B T}}$$

The populations of several ro-vibrational levels relative to the ground state were calculated for LTE and compared to those in this work. A sample of these values in the high temperature, high density regime is presented in Table 2. The index value represents the ordered rank of the ro-vibrational level by energy, where index 0 refers to (0,0), the para-H<sub>2</sub> ground state.

Table 2. Comparison of level populations relative to the ground state,  $N(v,j)/N(0,1)$ , at  $T = 10,000$  K and  $n_H = 10^8$  cm<sup>-3</sup>.

<i>index</i>	<i>v,j</i>	Steady state	LTE
5	0,5	2.901	2.904
10	1,1	0.549	0.550
29	2,5	0.924	0.930
41	3,3	0.396	0.400
55	4,1	0.111	0.112
100	6,3	0.0987	0.100
296	14,3	0.0130	0.0133

At low temperatures, the steady state level populations are only similar to LTE populations for the first few ro-vibrational levels. Even at the highest density considered,  $n_H = 10^8$  cm<sup>-3</sup>, the level populations are not even close to LTE at  $T = 1000$  K. By  $T = 5000$  K, however, the high density cases do match up with LTE. The departures from LTE decrease on average as temperature increases. At a given temperature, the departures from LTE are larger for higher energy levels. For the



highest temperatures and densities, these departures are quite small; the uppermost levels are within about 3% of LTE. It appears that the He-H<sub>2</sub> systems considered here cannot be approximated by LTE except for high densities and  $T \geq 5000$  K.

### Cooling

The cooling function was calculated in the temperature range  $500 \leq T \leq 20,000$  K and for densities  $1 \leq n_{\text{H}} \leq 10^8$  cm<sup>-3</sup>. It only includes the effects (excitation and de-excitation) collisions with helium atoms have on the H<sub>2</sub> ro-vibrational level populations. Hydrogen molecules and atoms are other likely collision partners in real astrophysical situations, and their effects would have to be included for a complete calculation of the cooling function. The purpose of this study was to compute the contribution of He collisions to the cooling function.

The results are presented in Figure 17. The points labeled “LTE” represent the cooling function in local thermodynamic equilibrium, calculated from H<sub>2</sub> level populations determined from the Boltzmann distribution. For high temperatures and densities of  $10^7$  and  $10^8$  cm<sup>-3</sup>, the cooling from He matches that in LTE.

The cooling function calculated in this work was compared, as seen in Figure 18, with that computed in Le Bourlot *et al.* (1999) for  $500 \leq T \leq 10,000$  K and  $n_{\text{H}} = 10$  cm<sup>-3</sup>. (The Le Bourlot data points were extracted from NASA ADS using Dexter.) The Le Bourlot cooling function is also that due only to collisions with helium atoms. The cooling function from this work is slightly larger at higher temperatures. The Le Bourlot study included vibrational levels only up to  $v = 3$  and a

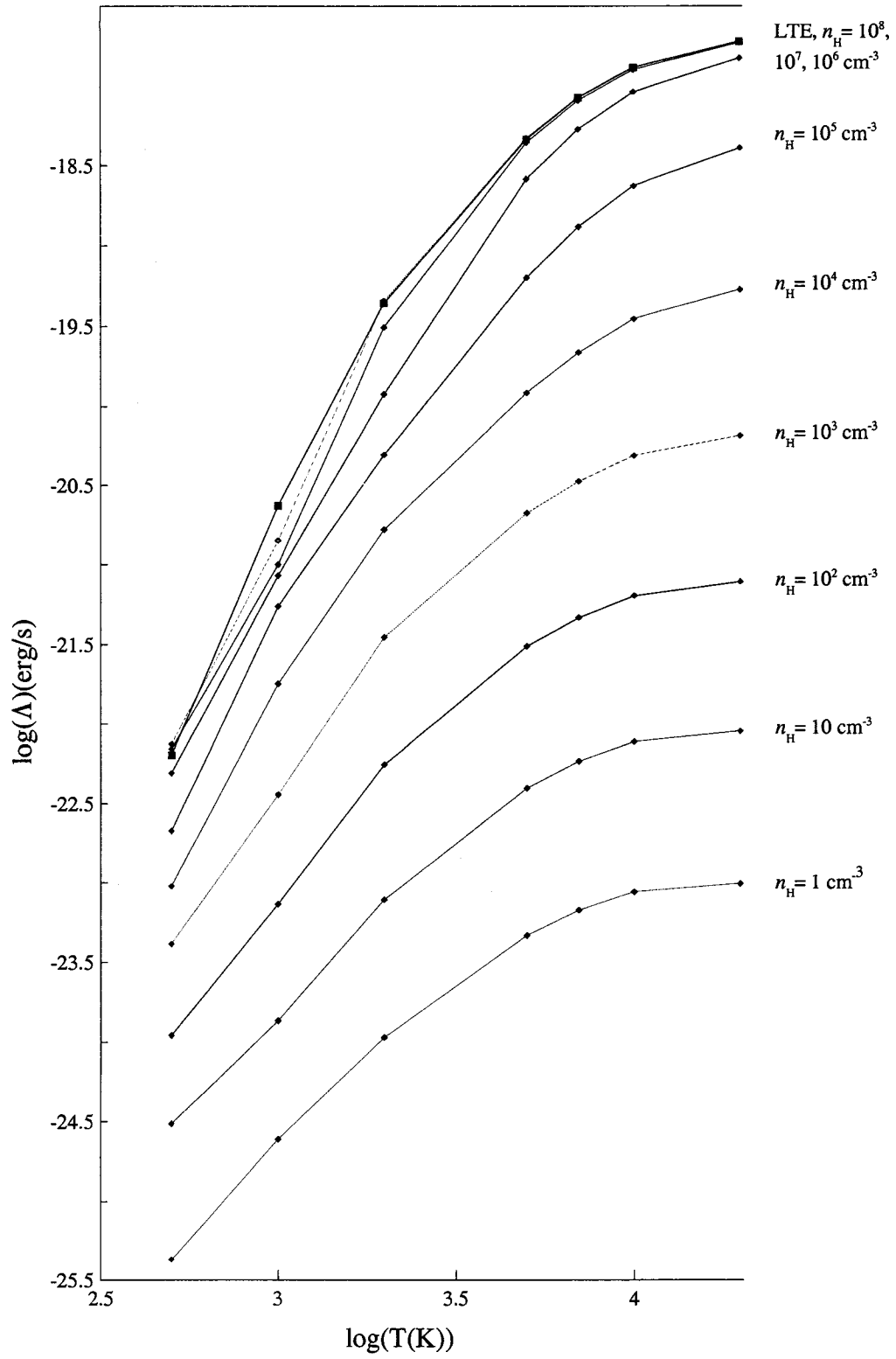


Figure 17. The cooling function  $\Lambda$ ;  $n_{\text{He}} = 0.1 n_{\text{H}}$ .

limited set of  $j$ -values corresponding to approximately the first 50 ro-vibrational levels; this study included all 301 ro-vibrational levels. However, it is not likely that the difference in cooling functions is due to the inclusion of higher levels because those levels are only sparsely populated at  $n_{\text{H}} = 10 \text{ cm}^{-3}$ ; the cooling comes mostly from spontaneous transitions out of the lower levels. It is more likely that the cooling function calculated in this work is higher because the majority of rate coefficients in this work were higher than those from Flower *et al.* (1998), which were used in the Le Bourlot study.

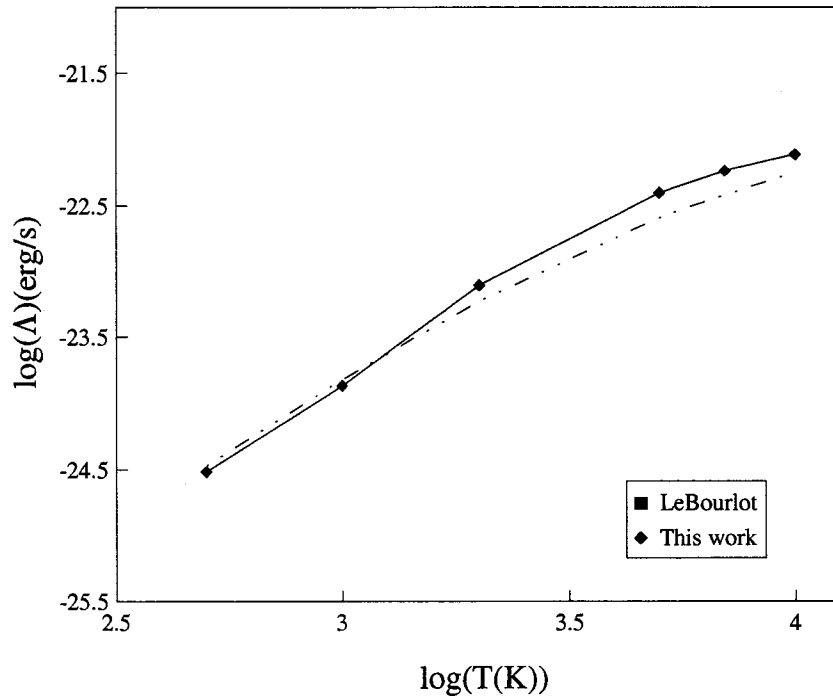


Figure 18. Cooling function at  $n_{\text{H}} = 10 \text{ cm}^{-3}$ ;  $n_{\text{He}} = 0.1 n_{\text{H}}$ .

## CHAPTER 4

### CONCLUSION

In this study, the rate coefficients for H<sub>2</sub> ro-vibrational transitions induced by He collisions were calculated using the semi-classical method. These were compared with corresponding rate coefficients computed using quantum mechanical methods. The semi-classical method yields good results for high temperatures and for pure rotational transitions, but is unreliable at low temperatures, especially concerning ro-vibrational transitions.

The cooling function for a wide range of temperature and density was presented. Good agreement was found when compared with the calculation of Le Bourlot *et al.* (1999) at  $n_{\text{H}} = 10 \text{ cm}^{-3}$ . The cooling function is less than that calculated under thermodynamic equilibrium conditions except for high temperatures and densities.

In order to interpret the spectral observations of molecular hydrogen emissions, rate coefficients describing the collisions which preclude emission must be known. It most likely cannot be assumed that the gas cloud is in thermal equilibrium except for regions of very high temperature and density. Cooling by helium atoms is important in many astrophysical regions, especially in clouds where most or all of the hydrogen is in molecular form. A quantum mechanical treatment would be best if possible, but a semi-classical study may be suitable at high temperatures.

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