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Calculated rotational and vibrational excitation rates for electron–HeH^+ collisions

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ABSTRACT

Molecular **R**-matrix calculations are performed at a range of energies to give rotational and vibrational excitation and de-excitation cross-sections and, hence, rates for electron collisions with HeH^+ up to electron temperatures of 20 000 K. Critical electron densities are also given. The rotational calculations include the Coulomb–Born completion of the cross-sections for high l values. Rates for the transition $j = 0 \rightarrow 2$, which have previously been assumed to be negligible, are found to be up to half those for $j = 0 \rightarrow 1$, raising the prospect of observing the HeH^+ $j = 2 \rightarrow 1$ emission line at 74.8 μm.

Key words: molecular data – molecular processes.

1 INTRODUCTION

It has long been suggested (Black 1978; Dabrowski & Herzberg (1978); Flower & Roueff 1979; Roberge & Dalgarno 1982; Dalgarno & Lepp 1987; Cecchi-Pestellini & Dalgarno 1993; Dubrovich & Lipovka 1995) that HeH^+ should be an important component in a number of astronomical environments. Particular attention has focused on the planetary nebula NGC 7027 (Roberge & Dalgarno 1982; Cecchi-Pestellini & Dalgarno 1993). Attempts to observe vibrational emission by Moorhead et al. (1988) proved negative. Recently, *ISO* has raised the possibility of observing a rotational emission spectrum. Preliminary results by Liu et al. (1996) found an emission feature at 149.23 μm which corresponds to the wavelength of the $j = 1 \rightarrow 0$ pure rotational transition; however, a more thorough analysis suggested that most, if not all of this feature, was actually caused by CH (Liu et al. 1997). Thus far the only astronomical detection of HeH^+ is a tentative one in the remnant of supernova 1987a (Miller et al. 1992).

HeH^+ is presumed to occur in diffuse ionizing environments. In these circumstances it is expected that, because of its large dipole moment, HeH^+ will be radiatively cooled and be present predominantly in its rotational and vibrational ground state. In this case, the flux of any observed emission spectrum will be governed by rates of collisional excitation. As electrons have very large collision cross-sections with molecular ions, it is generally assumed that even when the electron density, N_e, is only 10^{-4} that of molecular hydrogen, collisions with electrons dominate the excitation process.

There are essentially no experimental determinations of electron-impact excitation rates for molecular ions, so astronomical models have relied exclusively on theoretical estimates for these parameters. The standard methods for obtaining these parameters have been the Coulomb–Born approximation (Boĭkova & Ob''edkov 1968; Chu & Dalgarno 1974; Flower 1979; Neufeld & Dalgarno 1989) and classical-path perturbative methods (Faisal 1971; Dickinson & Muñoz 1977; Strekalov 1979; Dickinson & Flower 1981). These methods assume that the collisional excitation rate is determined solely by long-range effects and, for HeH^+, it has always been assumed that only dipolar interactions need be considered. Within these models only single jumps in vibrational or rotational quanta are allowed, leading to the conclusion that there are only three candidate HeH^+ emission lines at 149.23, 3.364 and 3.608 μm (Cecchi-Pestellini & Dalgarno 1993).

Work by us has suggested that the (dipole) Coulomb–Born approximation is not a reliable method for computing either vibrational (Sarpal & Tennyson 1993) or rotational (Rabadán, Sarpal & Tennyson 1998, henceforth RST98) electron-impact excitation rates. In particular, our most recent work, RST98, suggests that a more complete treatment can lead to significant population of the $j = 2$ rotational state. In this work we present vibrational and rotational electron-impact excitation rates for HeH^+ that should be significantly more reliable than those given by the (dipole) Coulomb–Born approximation.

2 CALCULATIONS

2.1 R-matrix calculations

In this work, we use the wavefunctions obtained by Sarpal et al. (1991a,b) using the UK molecular **R**-matrix package (Gillan, Tennyson & Burke 1995) to study electron scattering by HeH^+. The calculations were performed at 13 internuclear lengths in the range 1.0 to 4.0 a_0, including the equilibrium one at $R_e = 1.455\ a_0$. They used an inner region of 10 a_0. Total wavefunctions were based on a close-coupling expansion, which included the three lowest electronic states of HeH^+ represented via configuration interaction

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expansions. The close-coupling expansion was augmented by terms representing correlation and polarization effects. The continuum was represented by numerically calculated orbitals with $l \leq 5$, $m \leq 3$ and energy below 10 Ryd. These calculations were performed for four total symmetries: $^2\Sigma^+$, $^2\Pi$, $^2\Delta$ and $^2\Phi$. Each of these calculations produced a fixed-nuclei (FN) **T**-matrix.

2.2 Vibrational cross-sections

Vibrational excitation cross-sections have been calculated by us previously (Sarpal et al. 1991b; Sarpal & Tennyson 1993) using a number of models. The most sophisticated of these models (Sarpal et al. 1991b) used a full non-adiabatic treatment of the nuclear motion problem. The non-adiabatic treatment gives cross-sections with a rich and complicated resonance structure. The resonances are all very narrow and their effect, when calculating rates, is smeared out by the Maxwellian distribution of electron energies. We have estimated the effect of these resonances on the vibrational excitation rates as less than 10 per cent (Sarpal & Tennyson 1993).

In this work an adiabatic approximation was used to introduce the vibrational motion of the nuclei. This consists of vibrationally averaging the FN **T**-matrices. The necessary vibrational functions were obtained by numerically solving (LeRoy 1996) the Schrödinger equation in the *ab initio* ground state of HeH^+.

2.3 Rotational cross-sections

RST98 used the same HeH^+ **T**-matrices to perform a series of rotational calculations on HeH^+ using several models. These models included the use of FN **T**-matrices, adiabatic **T**-matrices, non-adiabatic **T**-matrices and the Coulomb–Born approximation. The work shows that a simple fixed-nuclei calculation produces results that are almost identical to the adiabatic model and similar to the more complicated non-adiabatic model. Furthermore, these results were substantially different from the pure Coulomb–Born cross-sections, demonstrating the importance of short-range effects in this kind of collision.

As in the vibrational excitation case, the non-adiabatic model shows a rich structure in the cross-section because of the presence of Rydberg states. The resonances are again very narrow and their importance, when calculating rates, appears to be small. Thus, in this work the simple fixed-nuclei model is used to obtain rates and critical densities for several rotation transitions.

Full details about the calculation of the rotational cross-sections used can be found in RST98. We summarize here the main points.

(i) The FN **T**-matrices are frame-transformed from the body frame to the laboratory frame. Rotational cross-sections for low-l partial waves are then obtained.

(ii) The Coulomb–Born (CB) approximation is evaluated to obtain the CB cross-section for the high-l waves not included in the FN **T**-matrices.

(iii) The sum of the previous two cross-sections produces the total one.

(iv) The known unphysical behaviour of the cross-sections at threshold, common in adiabatic nuclear rotation theories, is corrected using a simple kinematic ratio (Chandra & Temkin 1976).

(v) Significant cross-sections were found for rotational transitions with both $\Delta j = 1$ and $\Delta j = 2$. Cross-sections for $\Delta j = 3$ and $\Delta j = 4$ were found to be very small for HeH^+ and will not be considered further here.

Finally, it should be noted that the kinematic correction used can lead to cross-sections which do not obey detailed balance. To avoid this, we compute de-excitation rates from the excitation rates, obtained using threshold-corrected cross-sections, using detailed balance.

3 RESULTS AND DISCUSSION

3.1 Rotational transition rates

The rotational cross-sections were calculated in the range $E_{\mathrm{min}} = 0.001$ $\mathrm{E_h}$ up to $E_{\mathrm{max}} = 0.2$ $\mathrm{E_h}$. Rate coefficients for relatively low temperatures (<2000 K) have a small contribution from electron energies lower than E_{min}. To estimate and include that contribution, we have fitted the rotational excitation cross-sections between 0.001 and 0.037 $\mathrm{E_h}$ to the functional form

$$\sigma(E) = \sqrt{\frac{E - E_{\mathrm{th}}}{E}}\frac{a_l}{E^{b_l}}, \tag{1}$$

which includes the threshold correction, where E_{th} is the threshold energy. For σ in a_0^2 and E in Hartree, we obtained $b_l = 0.8$ for $|\Delta j = 1|$ transitions and $b_l = 1$ for $|\Delta j = 2|$; while $a_l = 14.9$ for $j = 0 \longrightarrow 1$, $a_l = 8.2$ for $j{=}1 \longrightarrow 2$ and $a_l = 3.3$ for $j{=}0 \longrightarrow 2$. On the other hand, the higher temperatures considered in this paper (15 000 and 20 000 K) have a small contribution from even higher energy electrons. To obtain the high-energy cross-sections needed, we fitted the cross-sections between 0.037 and 0.2 $\mathrm{E_h}$ to the form

$$\sigma(E) = \frac{a_h}{E^{b_h}} \tag{2}$$

and used the parameters to obtain cross-sections for the tail of the Maxwellian with $E > 0.2$ $\mathrm{E_h}$. We find $b_h = 0.8$ for $|\Delta j = 1|$ and $b_h = 1.0$ for $|\Delta j = 2|$ while $a_h = 18.5$ for $j = 0 \longrightarrow 1$; $a_h = 10.2$ for $j = 1 \longrightarrow 2$ and $a_h = 3.3$ for $j = 0 \longrightarrow 2$.

The rate coefficients were calculated assuming a Maxwellian distribution of electron energies. As a function of temperature (T), it reads as

$$\begin{aligned} q(T) = {} & 8\pi\left(\frac{1}{2\pi kT}\right)^{3/2} m_{\mathrm{e}}^{-1/2} \\ & \times \left[a_l \int_{E_{\mathrm{th}}}^{E_{\mathrm{min}}} \sqrt{E - E_{\mathrm{th}}}E^{3/2-b_l} \exp(-E/kT)\mathrm{d}E \right. \\ & + \int_{E_{\mathrm{min}}}^{E_{\mathrm{max}}} E\sigma(E) \exp(-E/kT)\ \mathrm{d}E \\ & \left. + \ a_h \int_{E_{\mathrm{max}}}^{\infty} E^{1-b_h} \exp(-E/kT)\mathrm{d}E \right], \end{aligned} \tag{3}$$

where k is the Boltzmann constant and m_{e} the electron mass. The first term on the right-hand side is the contribution from the low-energy electrons and it is evaluated from the a_l and b_l parameters of equation (1). The third term is the high-energy contribution and is evaluated from the a_h and b_h parameters of equation (2).

Rates for the rotational transitions involving $j = 0$, 1 and 2 are given in Table 1. We observe that for the excitation processes the rates peak between 500 and 1000 K. In all the cases, the cold electron contribution is significant under 2000 K (5 per cent of the tabulated values) and increases rapidly as the temperature decreases. In contrast, the tail contribution is only important for 15 000 and 20 000 K and is smaller than 7 per cent of the value given in the table. Furthermore, test calculations which used $E_{\mathrm{max}} = 0.37$ $\mathrm{E_h}$ gave results very similar to those presented here.

Pure CB calculation, as used previously (Chu & Dalgarno 1974; Neufeld & Dalgarno 1989) gives rates for $j = 0 \longrightarrow 1$ about 10 per

Table 1. Rate coefficients (cm^3 s^{-1}) for rotational transitions of HeH$^+$ by thermal electrons. Powers of 10 are given in parentheses.

T(K)	$j=0\rightarrow 1$	$j=0\rightarrow 2$	$j=1\rightarrow 0$	$j=1\rightarrow 2$	$j=2\rightarrow 0$	$j=2\rightarrow 1$
100	5.2(-7)	4.6(-8)	4.6(-7)	1.1(-7)	1.7(-7)	4.6(-7)
200	7.2(-7)	1.7(-7)	3.9(-7)	2.4(-7)	1.5(-7)	3.8(-7)
300	7.6(-7)	2.5(-7)	3.5(-7)	3.1(-7)	1.3(-7)	3.5(-7)
400	7.6(-7)	3.0(-7)	3.2(-7)	3.4(-7)	1.2(-7)	3.3(-7)
500	7.5(-7)	3.2(-7)	3.0(-7)	3.5(-7)	1.2(-7)	3.1(-7)
1000	6.9(-7)	3.5(-7)	2.5(-7)	3.6(-7)	9.3(-8)	2.6(-7)
2000	5.9(-7)	3.1(-7)	2.1(-7)	3.3(-7)	7.2(-8)	2.2(-7)
3000	5.4(-7)	2.8(-7)	1.9(-7)	3.0(-7)	6.1(-8)	1.9(-7)
4000	5.0(-7)	2.5(-7)	1.7(-7)	2.8(-7)	5.4(-8)	1.8(-7)
5000	4.8(-7)	2.3(-7)	1.6(-7)	2.7(-7)	4.9(-8)	1.7(-7)
6000	4.5(-7)	2.2(-7)	1.5(-7)	2.6(-7)	4.5(-8)	1.6(-7)
7000	4.4(-7)	2.0(-7)	1.5(-7)	2.5(-7)	4.2(-8)	1.5(-7)
8000	4.2(-7)	1.9(-7)	1.4(-7)	2.4(-7)	4.0(-8)	1.5(-7)
9000	4.1(-7)	1.8(-7)	1.4(-7)	2.4(-7)	3.8(-8)	1.4(-7)
10000	4.0(-7)	1.7(-7)	1.3(-7)	2.3(-7)	3.6(-8)	1.4(-7)
15000	3.6(-7)	1.5(-7)	1.2(-7)	2.1(-7)	3.0(-8)	1.3(-7)
20000	3.3(-7)	1.3(-7)	1.1(-7)	1.9(-7)	2.6(-8)	1.2(-7)

Table 2. Critical electron density (cm^{-3}), as a function of temperature, for rotational levels. Powers of 10 are given in parentheses.

T(K)	$j=1$	$j=2$
100	1.9(5)	5.1(6)
200	2.3(5)	5.8(6)
300	2.5(5)	6.4(6)
400	2.7(5)	6.8(6)
500	2.9(5)	7.3(6)
1000	3.5(5)	9.1(6)
2000	4.2(5)	1.2(7)
3000	4.7(5)	1.4(7)
4000	5.1(5)	1.6(7)
5000	5.4(5)	1.7(7)
6000	5.7(5)	1.9(7)
7000	5.9(5)	2.0(7)
8000	6.2(5)	2.1(7)
9000	6.4(5)	2.2(7)
10000	6.6(5)	2.3(7)
15000	7.3(5)	2.8(7)
20000	7.9(5)	3.3(7)

cent smaller than those given here. This is due to a cancellation of errors: on one side the inclusion of short-range effects in the CC+CB calculation increases the rotational rates, but part of this increase is compensated for by the threshold correction, which lowers the low-energy rotational cross-sections.

$|\Delta j = 2|$ transition rates from pure CB calculations are, however, in disagreement with our results. This is because the low-l partial wave contribution to the rotational cross-sections is dominant and is not well treated by simple CB theory.

The critical electron density is given as the ratio between the Einstein coefficient (A) of the excited state and the rate for the collisional de-excitation. We calculate A using the formulae[1] of Neufeld & Dalgarno (1989) and the *ab initio* vibrational functions and dipole function obtained in Sarpal et al. (1991b). Our values agree within 10 per cent with those by Neufeld & Dalgarno (1989), who based their estimates on the data of Dabrowski & Herzberg (1978). Critical densities are then obtained by

$$n_{\mathrm{cr}}(\alpha'; T) = \frac{A(\alpha' \rightarrow \alpha)}{q_{\alpha' \rightarrow \alpha}(T)} \; . \tag{4}$$

Tabulated values for the rotational excited states are given in Table 2. Results for $j = 2$ include the de-excitation to $j = 1$ and $j = 0$.

3.2 Vibrational transition rates

The vibrational excitation cross-sections were obtained directly from the adiabatic **T**-matrices of Sarpal et al. (1991b). As in the rotational case, the maximum energy was $E_{\mathrm{max}} = 0.2\ \mathrm{E_h}$. In order to calculate the tail contribution of the high-energy electrons, these cross-sections were also extrapolated as in the rotational case. The extrapolation parameters used in the vibrational excitation case were $a_l = E_{\mathrm{max}}\sigma(E_{\mathrm{max}})$ and $b_l = 1$. As the high-l contribution to the cross-sections is small, it was not necessary to use the CB approximation to augment the **R**-matrix calculations. In this case, the tail was never larger than 25 per cent of the total value. The rates for several vibrational transitions are given in Table 3.

The critical density values are obtained using equation (4). They are given in Table 4. Results for $v = 2$ include the de-excitation to $v = 1$ and $v = 0$.

We have fitted the tabulated rotational and vibrational parameters, both rates and critical densities, to the equation

$$f(T) = a(T/\mathrm{K})^b \exp(c/T). \tag{5}$$

The values obtained for these parameters, in the various transitions considered, are summarized in Table 5.

4 CONCLUSIONS

We have calculated rates and critical electron densities for several rotational and vibrational transitions of HeH$^+$ by electron impact for a range of temperatures.[2] The rotational calculations contain

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[1] Equation (13) of Neufeld & Dalgarno (1989) must be corrected by replacing $(2J + 1)$ by $(2J' + 1)$ in the denominator.

Table 3. Rate coefficients (cm^3 s^{-1}) for vibrational transitions of HeH$^+$ by thermal electrons. Powers of 10 are given in parentheses.

T(K)	$v = 0 \to 1$	$v = 0 \to 2$	$v = 1 \to 0$	$v = 1 \to 2$	$v = 2 \to 0$	$v = 2 \to 1$
100	2.5(-27)	1.0(-45)	5.1(-8)	4.8(-25)	5.3(-9)	1.2(-7)
200	1.1(-17)	1.8(-27)	4.9(-8)	1.9(-16)	4.2(-9)	9.6(-8)
300	1.6(-14)	2.0(-31)	4.3(-8)	1.3(-13)	3.5(-9)	8.0(-8)
400	5.7(-13)	2.0(-21)	3.8(-8)	3.1(-12)	3.0(-9)	7.0(-8)
500	4.8(-12)	1.2(-16)	3.5(-8)	2.1(-11)	2.7(-9)	6.3(-8)
1000	2.9(-10)	4.1(-13)	2.5(-8)	8.1(-10)	1.9(-9)	4.5(-8)
2000	1.9(-9)	2.0(-11)	1.8(-8)	4.2(-9)	1.3(-9)	3.2(-8)
3000	3.3(-9)	6.5(-11)	1.4(-8)	6.7(-9)	1.1(-9)	2.6(-8)
4000	4.1(-9)	1.1(-10)	1.2(-8)	8.1(-9)	9.3(-10)	2.2(-8)
5000	4.5(-9)	1.5(-10)	1.1(-8)	8.8(-9)	8.2(-10)	2.0(-8)
6000	4.8(-9)	1.8(-10)	1.0(-8)	9.2(-9)	7.4(-10)	1.8(-8)
7000	4.9(-9)	2.0(-10)	9.2(-9)	9.3(-9)	6.8(-10)	1.7(-8)
8000	4.9(-9)	2.2(-10)	8.6(-9)	9.3(-9)	6.3(-10)	1.5(-8)
9000	4.9(-9)	2.3(-10)	8.0(-9)	9.3(-9)	5.9(-10)	1.4(-8)
10000	4.9(-9)	2.4(-10)	7.6(-9)	9.2(-9)	5.5(-10)	1.4(-8)
15000	4.5(-9)	2.5(-10)	6.1(-9)	8.4(-9)	4.4(-10)	1.1(-8)
20000	4.1(-9)	2.4(-10)	5.2(-9)	7.7(-9)	3.7(-10)	9.4(-9)

Table 4. Critical electron density (cm^{-3}), as a function of temperature, for vibrational levels. Powers of 10 are given in parentheses.

T(K)	$v = 1$	$v = 2$
100	1.9(10)	1.3(10)
200	1.9(10)	1.6(10)
300	2.2(10)	2.0(10)
400	2.5(10)	2.2(10)
500	2.7(10)	2.5(10)
1000	3.7(10)	3.5(10)
2000	5.3(10)	5.0(10)
3000	6.5(10)	6.1(10)
4000	7.6(10)	7.1(10)
5000	8.5(10)	8.0(10)
6000	9.4(10)	8.7(10)
7000	1.0(11)	9.5(10)
8000	1.1(11)	1.0(11)
9000	1.2(11)	1.1(11)
10000	1.2(11)	1.1(11)
15000	1.5(11)	1.4(11)
20000	1.8(11)	1.7(11)

both short-range (from the **R**-matrix calculations) and long-range (CB approximation) effects. These data will be useful in the modelling of HeH$^+$ emission spectra in a number of environments.

One important result we find is that electron impact excitation can lead to direct population of the $j = 1$ and $j = 2$ rotationally excited states of HeH$^+$. Indeed, the excitation rate for $j = 0 \to 2$, previously assumed negligible, is found to be almost half that for $j = 0 \to 1$. This means that under favourable circumstances it should be possible to observe both the HeH$^+$ $j = 1$–0 and $j = 2$–1 rotational emission lines. Recent laboratory measurements gives these lines at wavelengths 149.137 and 74.7848 μm respectively (Matsushima, Oka & Takagi 1997). Observation of both lines would give a much more secure detection than observation of a single transition ever could.

Table 5. Fitted parameters of equation (8) to rates and critical electron densities in electron–HeH$^+$ collisions.

Transition	a (cm^3/s)	b	c (K)
	For transition rates		
$j = 0 \to 1$	5.2(-6)	-0.27	-1.0(2)
$j = 0 \to 2$	9.2(-6)	-0.42	-3.5(2)
$j = 1 \to 0$	1.7(-6)	-0.28	-5.3(1)
$j = 1 \to 2$	2.9(-6)	-0.27	-2.1(2)
$j = 2 \to 0$	1.5(-6)	-0.40	-4.1(1)
$j = 2 \to 1$	1.7(-6)	-0.27	-8.9(1)
$v = 0 \to 1$	1.4(-6)	-0.56	-4.6(3)
$v = 0 \to 2$	2.0(-7)	-0.64	-8.9(3)
$v = 1 \to 0$	1.1(-6)	-0.54	-5.0(1)
$v = 1 \to 2$	2.1(-6)	-0.54	-4.1(3)
$v = 2 \to 0$	9.4(-8)	-0.56	-3.6(1)
$v = 2 \to 1$	1.7(-6)	-0.52	-2.2(1)
	for critical densities		
$j = 1$	5.2(4)	0.27	2.2
$j = 2$	4.1(5)	0.44	6.5(1)
$v = 1$	7.7(8)	0.55	7.2(1)
$v = 2$	8.1(8)	0.52	4.5(1)

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[2] Extended versions of the tables given here are available on our server at http://www.tampa.phys.ucl.ac.uk/moldata

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