Rovibrational excitation of H_2 molecules by He atoms

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Abstract. We present the results of quantum mechanical calculations of cross sections and hence rate coefficients for rovibrational transitions in ortho- and para-H_2, induced by collisions with He. Rovibrational levels up to $(v, J) = (3, 8)$ were included in the calculations, and rate coefficients are available for temperatures $100 \leqslant T \leqslant 6000$ K. Comparison is made with previous calculations of rate coefficients for pure rotational transitions within the vibrational ground state and with measurements of the rate coefficient for vibrational relaxation $v = 1 \rightarrow 0$ at both high and low temperatures. Agreement is found to be good.

1. Introduction

Hydrogen and helium are by far the most abundant elements in the universe. Their relative abundance by number is approximately 10:1, and, when hydrogen is in molecular form, the ratio of H_2 to He is only 5:1. It follows that, after H_2 itself, He is the most abundant collision partner of molecular hydrogen in interstellar molecular clouds.

To date, the most refined and complete studies of the rotational excitation of H_2 by He are those of Schaefer and Köhler (1985). These authors used a then-recent determination of the He–H_2 interaction potential to calculate rotationally elastic and inelastic cross sections. Previous studies of He–H_2 collisions (Eastes and Secrest 1972, McGuire and Kouri 1974, Alexander and McGuire 1976) had relied on earlier determinations of the interaction potential, in which the van der Waals minimum was neglected.

Tsapline and Kutzelnigg (1973) were the first to compute the magnitude of the very shallow van der Waals minimum in the He–H_2 interaction potential. Coupled-channels calculations of rovibrational energy transfer, which incorporated the effects of this minimum, were subsequently performed for para-H_2 by Raczkowski *et al* (1978) and Orlikowski (1981). Near threshold, the van der Waals minimum tends to enhance the inelastic collision cross sections, as compared with results obtained using a purely repulsive potential (Flower and Kirkpatrick 1982a, b, Kirkpatrick 1982).

The He–H_2 potential has been the object of a much more recent study by Muchnick and Russek (1994), who also summarize the previous work on the HeH_2 system and give the terms of a parametric fit to their *ab initio* results. This fit was the starting point for the present computations of cross sections for the rovibrational excitation of H_2 by He, using the quantal coupled-channels method.

2. Numerical methods

The approach that we have followed here mirrors that of a recent study of H–H_2 collisions (Flower 1997). The quantal coupled-channels method was adopted (Flower 1990), using the programs developed by Launay (1977), amended to include the vibrational degree of freedom, and by Hutson and Green (1994). The code of Launay employs the de Vogelaere method to propagate the coupled, second-order differential equations, whereas that of Hutson and Green incorporates several alternatives, of which the hybrid modified log-derivative/Airy propagator (Alexander and Manolopoulos 1987) and the R-matrix propagator (Stechel *et al* 1978) methods were tried, with mutually consistent results. The precision of the cross sections is determined by the basis set size and is lowest at the outer edge of the basis, i.e. for the states of highest energy. We have included all the rovibrational levels (v, J) of H_2 with energies up to approximately 20 000 K relative to the $(0, 0)$ state. Thus, the highest energy level of ortho-H_2 was $(3, 7)$ and of para-H_2 was $(3, 8)$. Sufficient partial waves were computed at each collision energy to converge even the elastic cross sections to better than 1 part in 10^3. Results were obtained on a grid of about 50 energies extending up to 60 000 K (1 cm^{-1} ≡ 1.4388 K).

We compared the results of completely independent calculations, using the amended code of Launay (1977) and the MOLSCAT program of Hutson and Green (1994), for a subset of the collision energies. The same (Muchnick and Russek 1994) interaction potential was used throughout. The cross sections were found to agree to within, typically, a few per cent. We are thus confident of the accuracy of the numerical values that we have obtained.

For the purposes of the collision calculations, the interaction potential is most conveniently expressed in the form

$$V(\mathbf{r}, \mathbf{R}) = \sum_\lambda v_\lambda(r, R) \, P_\lambda(\hat{\mathbf{r}} \cdot \hat{\mathbf{R}}) \tag{1}$$

where $\mathbf{r}$ is the vector which connects the protons of the H_2 molecule, $\mathbf{R}$ is directed from the centre of mass (mid-point) of the molecule to the He atom and P_λ is the Legendre polynomial of order λ. Required for the scattering calculations are the matrix elements

$$y_\lambda(vJ, v'J'|R) = \int_0^\infty \chi^*(vJ|r) \, v_\lambda(r, R) \, \chi(v'J'|r) \, \mathrm{d}r \tag{2}$$

where the vibrational eigenfunctions $\chi(r)$ are taken to be harmonic oscillator wavefunctions (i.e. independent of J), adapted to the H_2 molecule (cf Eastes and Secrest 1972). The energies of the rovibrational levels, on the other hand, are taken from Dabrowski (1984) and are the measured values.

Muchnick and Russek (1994) do not present their results in the form of the Legendre polynomial expansion (1) above. Accordingly, we have projected out the Legendre polynomials up to $\lambda = 12$ for a grid of values of r and R. The number of angles $\mathbf{r} \cdot \mathbf{R}$ was sufficient to ensure the convergence of these scalar products, in the sense that the terms $v(r, R)$ with λ odd were very small compared with those with λ even (the odd λ contributions should vanish identically owing to the symmetry of the He–H_2 potential). Finally, the accuracy of the result was checked by regenerating the potential using equation (1) and comparing with the numerical values from the parametric fit of Muchnick and Russek (1994, table 2). In the subsequent collision calculations, terms with $\lambda = 0, 2, 4$ and 6 were retained in the potential expansion.

3. Results

In tables 1 and 2 we presented the values of the rate coefficients for selected transitions between levels of the $v = 0, 1$ and 2 states of para- and ortho-H$_2$ at three kinetic temperatures, $T = 1000, 2000$ and 4500 K; for comparison purposes, the latter were chosen to be the same as in the study (Flower 1997) of rovibrational transitions in H$_2$ induced by collisions with H. The rate coefficients, $q(T)$, for de-excitation were calculated from

$$q(T) = \left(\frac{8kT}{\pi\mu}\right)^{1/2} \int_0^\infty Q(x)x\,e^{-x}\,dx \qquad (3)$$

in which $Q(x)$ is the de-excitation cross section and $x = E/kT$; μ is the reduced mass of the He–H$_2$ system and E the barycentric collision energy, relative to the initial (upper) level. The integral was evaluated numerically, using a trapezoidal rule on a fine grid of the integration variable, x; $Q(x)$ was generated at the grid points by cubic spline interpolation of its computed values. Rate coefficients for excitation, also given in table 1, were obtained from the detailed balance relation

$$(2J + 1)q_{J\to J'}(T) = (2J' + 1)q_{J'\to J}(T)\exp[-(E_{J'} - E_J)/kT]. \qquad (4)$$

In table 3, we present the computed values of the relaxation rate coefficient in the temperature range $100 \leqslant T \leqslant 3000$ K. It has been evaluated as

$$q_{v=1\to 0}(T) = \frac{\sum_{JJ'} n(v = 1, J)\,q(v = 1, J \to v' = 0, J')}{\sum_J n(v = 1, J)} \qquad (5)$$

where q denotes a rate coefficient for de-excitation from $v = 1, J$ to $v' = 0, J'$ and $n(v = 1, J)$ is the population of the upper level of the collision-induced transition. For the latter, we assume a Boltzmann distribution to be established amongst the rotational levels of the $v = 1$ vibrational state.

The rate constant for the vibrational relaxation of H$_2(v = 1)$ in He has been measured by Audibert *et al* (1976), for both para- and ortho-H$_2$, and, at higher temperatures and for normal H$_2$, by Dove and Teitelbaum (1974). The measurements of Audibert *et al* show the relaxation rate coefficient for para-H$_2$ to be below that for ortho-H$_2$ at $T = 50$ K, with the two values approaching each other and becoming equal, to within the experimental error bar, at $T = 296$ K. We see from table 3 that the trend of the theoretical results is in agreement with the measurements of Audibert *et al*, with the values for para-H$_2$ falling below those for ortho-H$_2$ as T decreases. At $T = 100$ K, we find that the calculated relaxation rate coefficients lie approximately 30% and 40% above the experimental values for ortho- and para-H$_2$, respectively, as estimated from figure 3 of Audibert *et al*. At $T = 300$ K, the mean of the calculated values exceeds the measurements (indistinguishable for ortho and para) by a factor of 2. Shock tube experiments have been performed (Dove and Teitelbaum 1974), yielding results at high temperatures. At the highest temperature for which measurements were made, $T = 3000$ K, the computed relaxation rate exceeds that measured (for normal H$_2$) by a factor of 2. The agreement between the experimental and theoretical values improves towards lower temperatures (the measurements extended down to $T = 1350$ K). We consider this level of agreement with the results of both high- and low-temperature experiments, extending over a range of six decades in the values of the relaxation rate coefficient, to be encouraging.

At low temperatures, the low rotational levels of the $v = 1$ manifold are preferentially populated, with the higher rotational levels contributing increasingly as T rises. Thus, although the rotational relaxation rate coefficient is a thermally averaged quantity, its variation with temperature provides some discrimination amongst the rotational levels of

Table 1. Rate coefficients (in units of cm^3 s^{-1}) for rovibrational transitions in para-H$_2$, induced by He atom collisions. Results are given at three values of the kinetic temperature, T. The values of (v, J) which label the columns denote the initial state, those which label the rows denote the final state. Thus, the upper right triangle of each matrix refers to collisional de-excitation and the lower left triangle to excitation (obtained using the detailed balance relation, equation (4)). More extensive results are available electronically from the CCP7 server (ftp://ccp7.arm.ac.uk/ccp7/) or from david.flower@durham.ac.uk.

$T = 1000$ K

	(0, 0)	(0, 2)	(0, 4)	(0, 6)	(0, 8)	(1, 0)	(1, 2)	(1, 4)	(0, 10)	(1, 6)	(1, 8)	(2, 0)	(0, 12)	(2, 2)
(0, 0)	1.5D−09	1.5D−11	4.2D−13	1.1D−14	2.4D−16	3.6D−16	9.4D−17	3.7D−17	4.8D−18	7.8D−18	9.0D−19	4.4D−19	8.9D−20	3.0D−19
(0, 2)	4.4D−11	1.6D−09	9.3D−12	2.1D−13	4.7D−15	8.1D−16	8.6D−16	3.0D−16	9.8D−17	6.0D−17	7.5D−18	2.4D−18	1.9D−18	1.8D−18
(0, 4)	7.0D−13	5.2D−12	1.6D−09	3.6D−12	6.4D−14	1.1D−15	2.3D−15	1.4D−15	1.3D−15	3.3D−16	4.2D−17	2.3D−18	2.6D−17	4.9D−18
(0, 6)	4.3D−15	2.8D−14	8.7D−13	1.6D−09	1.4D−12	4.0D−16	1.3D−15	6.8D−15	2.0D−14	2.1D−14	1.6D−16	4.0D−18	3.6D−16	8.4D−18
(0, 8)	1.2D−17	7.8D−17	1.9D−15	1.7D−13	1.6D−09	4.7D−17	2.0D−16	6.4D−15	6.0D−13	1.6D−14	3.3D−15	2.0D−18	6.9D−15	6.4D−18
(1, 0)	9.1D−19	6.8D−19	1.6D−18	2.5D−18	2.4D−18	1.6D−09	1.6D−11	5.3D−13	5.5D−19	2.9D−13	4.1D−16	1.1D−15	4.2D−20	3.4D−16
(1, 2)	7.3D−19	2.2D−18	1.1D−17	2.5D−17	3.1D−17	5.0D−11	1.6D−09	1.1D−11	9.5D−18	4.6D−12	7.6D−15	2.6D−15	7.9D−19	2.8D−15
(1, 4)	1.7D−19	4.6D−19	3.9D−18	7.7D−17	5.9D−16	9.6D−13	6.5D−12	1.6D−09	1.4D−16	2.7D−14	9.6D−14	3.7D−15	1.1D−17	7.2D−15
(0, 10)	1.7D−20	1.2D−19	2.8D−18	1.8D−16	4.3D−14	7.9D−19	4.4D−18	1.1D−16	1.6D−09	1.9D−13	6.7D−14	3.6D−19	2.9D−13	1.1D−18
(1, 6)	9.4D−21	2.4D−20	2.4D−19	6.7D−18	5.2D−16	7.5D−15	4.5D−14	1.2D−12	9.2D−15	1.6D−09	1.9D−12	1.3D−15	2.1D−16	4.2D−15
(1, 8)	1.5D−22	4.2D−22	4.2D−21	1.3D−19	1.1D−17	2.8D−17	1.7D−16	3.5D−15	3.2D−15	2.6D−13	1.7D−09	1.6D−16	2.0D−14	6.3D−16
(2, 0)	3.9D−24	7.0D−24	1.2D−23	8.8D−23	3.6D−22	3.8D−18	3.0D−18	7.1D−18	8.8D−22	9.8D−18	8.3D−18	1.6D−09	5.7D−22	1.8D−11
(0, 12)	1.5D−23	1.0D−22	2.5D−21	1.5D−19	2.2D−17	2.7D−21	1.7D−20	3.8D−19	1.3D−14	2.8D−17	1.9D−16	1.0D−20	1.6D−09	4.0D−20
(2, 2)	8.4D−24	1.7D−23	8.2D−23	5.9D−22	3.6D−21	3.8D−18	1.0D−17	4.4D−17	8.9D−21	9.6D−17	1.0D−16	5.7D−11	6.8D−21	1.6D−09

$T = 2000$ K

	(0, 0)	(0, 2)	(0, 4)	(0, 6)	(0, 8)	(1, 0)	(1, 2)	(1, 4)	(0, 10)	(1, 6)	(1, 8)	(2, 0)	(0, 12)	(2, 2)
(0, 0)	2.0D−09	3.2D−11	1.9D−12	1.1D−13	5.3D−15	4.9D−15	1.9D−15	1.0D−15	2.2D−16	3.4D−16	6.7D−17	1.4D−17	8.5D−18	1.7D−17
(0, 2)	1.2D−10	2.1D−09	2.9D−11	1.5D−12	7.7D−14	9.4D−15	1.4D−14	7.3D−15	3.5D−15	2.3D−15	4.8D−16	8.4D−17	1.5D−16	9.2D−17
(0, 4)	7.3D−12	2.9D−11	2.2D−09	1.6D−11	6.9D−13	2.1D−14	2.7D−14	2.5D−14	3.3D−14	9.2D−15	2.0D−15	1.1D−16	1.4D−15	1.9D−16
(0, 6)	2.4D−13	8.8D−13	9.3D−12	2.2D−09	8.3D−12	1.3D−14	2.3D−14	6.9D−14	3.1D−13	3.9D−14	9.8D−15	2.1D−16	1.3D−14	2.5D−16
(0, 8)	4.9D−15	1.8D−14	1.6D−13	3.3D−12	2.2D−09	2.4D−14	5.7D−15	3.8D−14	4.5D−12	1.9D−13	5.7D−14	1.9D−16	1.5D−13	3.2D−16
(1, 0)	2.4D−16	1.2D−16	2.7D−16	2.8D−16	1.3D−16	2.1D−09	3.4D−11	2.3D−12	2.8D−17	1.4D−13	8.0D−15	1.2D−14	3.1D−18	5.7D−15
(1, 2)	3.8D−16	7.0D−16	1.4D−15	2.0D−15	1.2D−15	1.3D−10	2.1D−09	3.4D−11	3.3D−16	1.2D−11	3.0D−14	2.7D−14	4.4D−17	3.8D−14
(1, 4)	2.1D−16	3.8D−16	1.3D−15	6.2D−15	8.4D−15	9.1D−12	3.4D−11	2.2D−09	2.4D−15	1.9D−11	8.9D−14	6.1D−14	3.6D−16	7.6D−14
(0, 10)	6.2D−17	2.5D−16	2.3D−16	3.7D−14	1.3D−12	1.5D−16	3.3D−16	2.4D−15	2.2D−09	7.5D−14	4.9D−13	5.4D−17	3.6D−16	1.1D−16
(1, 6)	4.2D−17	7.5D−17	3.0D−16	2.1D−15	2.6D−14	3.6D−13	1.2D−11	2.5D−13	3.4D−14	2.2D−09	4.4D−12	2.2D−15	3.1D−15	6.5D−14
(1, 8)	3.6D−18	6.6D−18	2.8D−17	2.3D−16	3.3D−15	8.6D−15	3.0D−14	8.9D−14	2.5D−13	4.4D−12	1.7D−09	4.3D−16	5.6D−14	1.7D−14
(2, 0)	4.1D−20	6.5D−20	8.7D−20	2.7D−19	6.2D−19	7.2D−16	9.1D−16	6.1D−14	5.4D−17	2.2D−15	4.3D−16	2.2D−09	5.7D−18	3.6D−11
(0, 12)	5.4D−19	2.4D−18	2.4D−17	3.8D−16	1.5D−13	4.0D−18	4.4D−17	3.6D−16	3.6D−16	3.1D−15	5.6D−14	5.7D−18	2.2D−09	1.6D−17
(2, 2)	2.0D−19	2.8D−19	5.8D−19	1.3D−15	4.1D−18	1.3D−15	3.8D−14	7.6D−14	1.1D−16	6.5D−14	1.7D−14	1.4D−10	3.0D−18	2.1D−09

Table 1. Continued.

$T = 4500$ K

	(0, 0)	(0, 2)	(0, 4)	(0, 6)	(0, 8)	(1, 0)	(1, 2)	(1, 4)	(0, 10)	(1, 6)	(1, 8)	(2, 0)	(0, 12)	(2, 2)
(0, 0)	2.8D−09	6.2D−11	7.5D−12	9.7D−13	1.1D−13	6.7D−14	3.6D−14	2.4D−14	1.2D−14	1.2D−14	4.1D−15	7.3D−16	1.1D−15	7.8D−16
(0, 2)	2.8D−10	2.9D−09	7.9D−11	9.2D−12	1.1D−12	1.6D−13	2.1D−13	1.5D−13	1.2D−13	7.3D−14	2.5D−14	3.4D−15	1.2D−14	4.4D−15
(0, 4)	4.6D−11	1.1D−10	3.0D−10	5.8D−11	6.2D−12	3.0D−13	3.4D−13	3.6D−13	7.1D−13	2.0D−13	7.8D−14	7.2D−15	7.7D−14	8.4D−15
(0, 6)	5.8D−12	1.2D−11	5.6D−11	3.0D−09	4.0D−11	3.3D−13	3.9D−13	6.5D−13	3.9D−12	5.3D−13	2.4D−13	1.0D−14	4.3D−13	1.2D−14
(0, 8)	5.2D−13	1.2D−12	4.6D−12	3.1D−11	3.1D−09	1.5D−13	2.1D−13	4.7D−13	2.8D−11	1.4D−12	7.6D−13	1.3D−14	2.5D−12	1.4D−14
(1, 0)	1.8D−14	9.6D−15	1.3D−14	1.4D−14	8.5D−15	2.8D−09	6.4D−11	8.3D−12	2.8D−15	1.1D−12	1.4D−13	1.4D−13	6.8D−16	8.1D−14
(1, 2)	4.3D−14	5.5D−14	6.6D−14	7.7D−14	5.4D−14	2.9D−10	2.9D−09	8.4D−11	2.2D−14	1.1D−11	1.4D−12	3.8D−13	6.2D−15	4.6D−13
(1, 4)	4.0D−14	5.4D−14	9.6D−14	1.8D−13	1.7D−13	5.3D−11	1.2D−10	3.0D−09	8.2D−14	6.4D−11	7.3D−12	7.2D−13	2.9D−14	8.1D−13
(0, 10)	3.5D−14	8.4D−14	3.5D−13	2.0D−12	1.9D−11	3.3D−14	5.6D−14	1.5D−13	3.1D−09	5.9D−13	2.9D−12	7.6D−15	2.0D−11	1.0D−14
(1, 6)	1.9D−14	2.7D−14	5.4D−14	1.5D−13	4.9D−13	7.2D−12	1.5D−11	6.3D−11	3.2D−13	3.0D−09	4.5D−11	7.7D−13	1.2D−13	9.2D−13
(1, 8)	5.4D−15	7.4D−15	1.6D−14	5.2D−14	2.1D−13	7.0D−13	1.5D−12	5.7D−12	1.2D−12	3.6D−11	3.1D−09	3.7D−13	5.4D−13	5.1D−13
(2, 0)	5.5D−17	5.8D−17	8.7D−17	1.3D−16	2.0D−16	4.1D−14	2.4D−14	3.3D−14	1.9D−16	3.5D−14	2.1D−14	2.8D−09	1.7D−16	6.6D−11
(0, 12)	1.9D−15	4.9D−15	2.2D−14	1.2D−13	9.4D−13	4.5D−15	9.2D−15	3.0D−14	1.2D−11	1.3D−13	7.2D−13	3.9D−13	3.1D−09	6.4D−15
(2, 2)	2.7D−16	3.4D−16	4.6D−16	6.5D−16	1.0D−15	1.0D−13	1.3D−13	1.7D−13	1.1D−15	1.9D−13	1.3D−13	3.0D−10	1.2D−15	2.9D−09

Table 2. As for table 1 but for ortho-H_2.

$T = 1000$ K

	(0, 1)	(0, 3)	(0, 5)	(0, 7)	(1, 1)	(1, 3)	(0, 9)	(1, 5)	(0, 11)	(1, 7)	(2, 1)	(2, 3)	(1, 9)	(0, 13)
(0, 1)	1.2D−09	1.4D−11	3.5D−13	8.3D−15	5.8D−16	2.3D−16	1.8D−16	6.4D−17	3.5D−18	9.9D−18	1.1D−18	8.0D−19	9.4D−19	6.7D−20
(0, 3)	1.4D−11	1.6D−09	5.9D−12	1.2D−13	1.5D−15	1.1D−15	2.5D−15	3.2D−15	5.1D−17	5.1D−17	3.2D−18	2.6D−18	5.3D−18	1.0D−18
(0, 5)	1.2D−13	2.1D−12	1.6D−09	2.2D−12	1.0D−15	3.9D−15	3.5D−14	1.8D−15	6.8D−16	3.2D−16	4.3D−18	7.9D−18	3.3D−17	1.3D−17
(0, 7)	5.0D−16	7.0D−15	3.8D−13	1.6D−09	2.4D−16	2.6D−15	9.0D−13	1.2D−14	1.1D−14	2.7D−15	4.5D−18	1.8D−17	2.9D−16	2.0D−16
(1, 1)	1.5D−18	3.7D−18	7.1D−18	1.0D−17	1.6D−09	1.6D−11	6.1D−18	4.6D−13	8.7D−19	1.3D−14	1.8D−15	8.6D−16	3.2D−16	4.3D−20
(1, 3)	6.2D−19	3.0D−18	2.9D−17	1.2D−16	1.7D−11	1.6D−09	7.9D−17	7.2D−12	1.1D−17	1.7D−13	4.6D−15	3.7D−15	4.2D−15	5.8D−19
(0, 9)	1.0D−18	1.4D−17	5.6D−16	8.4D−14	1.4D−17	1.7D−16	1.7D−09	1.5D−14	4.1D−13	3.8D−14	1.4D−18	1.2D−17	3.8D−15	4.3D−15
(1, 5)	6.4D−20	3.3D−19	5.2D−18	2.0D−16	1.8D−13	2.7D−12	2.7D−15	1.7D−09	1.5D−14	2.9D−12	3.4D−15	1.2D−14	5.5D−14	8.1D−18
(0, 11)	1.1D−21	1.6D−20	6.0D−19	6.0D−17	1.1D−19	1.4D−18	2.3D−14	6.4D−17	2.0D−16	3.2D−14	1.1D−19	1.2D−18	1.1D−13	2.1D−13
(1, 7)	1.9D−21	9.8D−21	1.7D−19	8.7D−18	9.7D−16	1.2D−14	1.3D−15	5.5D−13	1.6D−09	1.7D−09	8.0D−16	7.7D−15	1.2D−12	1.7D−16
(2, 1)	1.0D−23	2.8D−23	1.1D−22	6.8D−22	6.5D−18	1.6D−17	2.2D−21	3.0D−17	1.9D−14	3.8D−17	1.6D−09	1.8D−11	2.1D−17	1.9D−21
(2, 3)	7.8D−24	2.5D−23	2.2D−22	2.8D−21	3.3D−18	1.4D−17	2.1D−20	1.1D−16	3.2D−21	4.0D−16	2.0D−11	1.7D−09	2.5D−16	2.2D−20
(1, 9)	1.9D−23	1.1D−22	1.9D−21	9.7D−20	2.6D−18	3.2D−17	1.4D−17	1.1D−15	3.7D−20	1.3D−13	4.8D−17	5.1D−16	1.6D−09	1.3D−14
(0, 13)	8.0D−25	1.2D−23	4.5D−22	4.0D−20	2.0D−22	2.6D−21	9.1D−18	9.6D−20	7.3D−15	1.0D−17	2.5D−21	2.7D−20	7.7D−15	1.6D−09

$T = 2000$ K

	(0, 1)	(0, 3)	(0, 5)	(0, 7)	(1, 1)	(1, 3)	(0, 9)	(1, 5)	(0, 11)	(1, 7)	(2, 1)	(2, 3)	(1, 9)	(0, 13)
(0, 1)	2.0D−09	3.6D−11	2.0D−12	1.1D−13	8.7D−15	5.1D−15	5.1D−15	2.1D−15	2.1D−16	5.3D−16	4.8D−17	5.3D−17	8.5D−17	8.1D−18
(0, 3)	5.5D−11	2.2D−09	2.2D−11	1.0D−12	1.7D−14	1.9D−14	5.1D−15	8.5D−15	2.3D−15	2.2D−15	1.3D−16	1.4D−16	3.8D−16	9.4D−17
(0, 5)	2.3D−12	1.6D−11	2.2D−09	1.1D−11	2.2D−14	4.2D−14	4.6D−13	3.1D−14	2.1D−14	9.6D−15	1.6D−16	3.0D−16	1.8D−15	9.1D−16
(0, 7)	6.0D−14	3.7D−13	5.5D−12	2.2D−09	8.2D−15	2.7D−14	6.1D−12	1.2D−13	2.1D−13	4.8D−14	2.6D−16	4.3D−16	9.8D−15	8.9D−15
(1, 1)	4.4D−16	5.7D−16	9.6D−16	7.5D−16	2.1D−09	4.0D−11	2.6D−16	2.5D−12	4.3D−17	1.5D−13	2.3D−14	1.5D−14	8.1D−15	4.3D−18
(1, 3)	4.0D−16	9.8D−16	2.9D−15	3.9D−15	6.2D−11	2.1D−09	1.8D−15	2.5D−11	3.6D−16	1.4D−12	4.9D−14	5.3D−14	7.5D−14	4.1D−17
(0, 9)	9.7D−16	6.3D−15	7.7D−14	2.1D−12	9.8D−16	4.2D−15	2.2D−09	5.6D−14	3.4D−12	3.1D−13	1.4D−16	4.0D−16	6.6D−14	1.0D−13
(1, 5)	1.3D−16	3.4D−16	1.7D−15	1.3D−14	3.0D−12	1.9D−11	1.8D−14	2.2D−09	2.9D−15	1.4D−11	6.3D−14	1.1D−13	6.4D−13	3.4D−16
(0, 11)	1.1D−17	7.4D−17	9.0D−16	1.9D−14	3.0D−12	1.9D−11	8.9D−13	2.3D−15	2.2D−09	8.1D−14	3.1D−17	1.3D−16	7.5D−13	3.4D−16
(1, 7)	1.6D−17	4.5D−17	2.6D−16	2.7D−15	9.4D−14	5.4D−13	5.1D−14	7.0D−12	5.1D−14	2.2D−09	2.5D−14	7.6D−14	7.6D−12	3.1D−15
(2, 1)	1.4D−19	2.5D−19	4.2D−19	1.4D−18	1.4D−15	1.9D−15	2.2D−18	3.1D−15	1.9D−18	2.4D−15	2.1D−09	4.4D−11	9.3D−16	4.0D−19
(2, 3)	2.5D−19	4.3D−19	1.3D−18	3.7D−18	1.5D−15	3.2D−15	1.0D−17	9.0D−15	1.3D−17	1.2D−14	7.0D−11	2.2D−09	5.8D−15	2.4D−18
(1, 9)	9.7D−19	2.8D−18	1.8D−17	2.0D−16	1.8D−15	1.1D−14	4.0D−15	1.2D−13	1.7D−13	2.8D−12	3.5D−15	1.4D−14	2.2D−09	5.0D−14
(0, 13)	8.4D−20	6.4D−19	8.3D−18	1.7D−16	8.9D−19	5.4D−18	5.7D−15	5.7D−17	4.4D−13	1.0D−15	1.4D−18	5.2D−18	4.5D−14	2.2D−09

Table 2. Continued.

$T = 4500$ K

	(0, 1)	(0, 3)	(0, 5)	(0, 7)	(1, 1)	(1, 3)	(0, 9)	(1, 5)	(0, 11)	(1, 7)	(2, 1)	(2, 3)	(1, 9)	(0, 13)
(0, 1)	2.9D−09	8.5D−11	1.0D−11	1.3D−12	1.4D−13	9.6D−14	1.4D−13	5.7D−14	1.4D−14	2.3D−14	2.2D−15	2.8D−15	6.9D−15	1.4D−15
(0, 3)	1.6D−10	3.0D−09	6.8D−11	7.6D−12	2.4D−13	2.8D−13	9.0D−13	1.8D−13	9.8D−14	7.8D−14	5.8D−15	7.0D−15	2.4D−14	1.0D−14
(0, 5)	2.2D−11	7.7D−11	3.0D−09	4.8D−11	3.6D−13	4.6D−13	4.9D−12	4.3D−13	5.5D−13	2.2D−13	9.2D−15	1.1D−14	7.6D−14	6.0D−14
(0, 7)	2.4D−12	7.4D−12	4.1D−11	3.0D−09	2.7D−13	4.2D−13	3.4D−11	9.4D−13	3.1D−12	6.4D−13	1.2D−14	1.4D−14	2.5D−13	3.4D−13
(1, 1)	3.6D−14	3.3D−14	4.4D−14	3.8D−14	2.9D−09	9.0D−11	1.8D−14	1.2D−11	5.1D−15	1.5D−12	3.0D−13	2.2D−13	1.8D−13	1.2D−15
(1, 3)	4.9D−14	7.5D−14	1.1D−13	1.2D−13	1.7D−10	2.9D−09	6.9D−14	7.4D−11	2.5D−14	8.9D−12	5.7D−13	6.4D−13	1.1D−12	6.8D−15
(0, 9)	1.9D−13	6.2D−13	3.0D−12	2.4D−11	8.9D−14	1.8D−13	3.1D−09	5.3D−13	2.4D−11	2.0D−12	1.1D−14	1.6D−14	9.0D−13	2.1D−12
(1, 5)	3.4D−14	5.5D−14	1.2D−13	3.0D−13	2.6D−11	8.5D−13	2.4D−13	3.0D−09	9.7D−14	5.4D−11	8.5D−13	1.1D−12	5.8D−12	3.1D−14
(0, 11)	1.2D−14	4.1D−14	2.0D−13	1.4D−12	1.6D−14	3.9D−14	1.5D−11	1.3D−13	3.1D−09	6.5D−13	7.7D−15	1.4D−14	4.0D−12	1.8D−11
(1, 7)	1.2D−14	2.1D−14	5.3D−14	1.8D−13	3.1D−12	9.0D−12	7.9D−13	4.7D−11	4.1D−13	3.0D−09	6.2D−13	9.7D−13	3.8D−11	1.3D−13
(2, 1)	1.7D−16	2.3D−16	3.2D−16	4.9D−16	8.6D−14	8.4D−14	6.3D−16	1.1D−13	7.1D−16	9.0D−14	2.9D−09	9.4D−11	5.3D−14	2.1D−16
(2, 3)	4.1D−16	5.4D−16	7.8D−16	1.1D−15	1.2D−13	1.8D−13	1.8D−15	2.7D−13	2.6D−15	2.8D−13	1.9D−10	2.9D−09	2.0D−13	6.6D−16
(1, 9)	2.6D−15	4.7D−15	1.3D−14	5.2D−14	2.6D−13	8.2D−13	2.6D−13	3.7D−12	1.9D−12	2.8D−11	2.7D−13	5.1D−13	3.1D−09	6.0D−13
(0, 13)	6.4D−16	2.4D−15	1.2D−14	8.0D−14	2.0D−15	5.9D−15	6.9D−13	2.4D−14	9.8D−12	1.1D−13	1.2D−15	2.0D−15	7.0D−13	3.1D−09

Table 3. Computed values of the rate coefficient (in units of cm^3 s^{-1}) for vibrational relaxation of $H_2(v = 1)$ in collisions with He atoms. For each value of the temperature, T, the upper entry is for ortho-H_2 and the lower entry for para-H_2. Numbers in parentheses are powers of 10.

T (K)	$q_{v=1 \to 0}$
100	1.3(−18)
	7.4(−19)
300	4.5(−17)
	5.1(−17)
500	5.1(−16)
	5.2(−16)
1000	1.2(−14)
	1.2(−14)
3000	1.1(−12)
	1.1(−12)

the excited vibrational state. In view of the overall level of agreement of the computed and experimental results, we consider the rate coefficients presented here to be the most accurate and complete that are currently available.

Cross sections and rate coefficients for pure rotational transitions within the ground vibrational state, $v = 0$, have been calculated by Schaefer (1985, personal communication). The rate coefficients for selected transitions were tabulated by Danby *et al* (1987), for comparison with their H_2–H_2 results. At $T = 500$ K, we find that the He–H_2 rate coefficients for transitions $v = 0$, $J \to J - 2$, $J \leqslant 6$, calculated by Schaefer agree with the present results to within a few per cent.

Acknowledgments

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