OXYGEN CHEMISTRY IN THE INTERSTELLAR MEDIUM: THE EFFECT OF VIBRATIONAL EXCITATION OF H_2 IN THE $O(^3P)+H_2$ REACTION

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ABSTRACT

The $O + H_2 \rightarrow OH + H$ reaction is considered to be the key step in initiating oxygen chemistry in shocked interstellar molecular clouds. We present extensive quantum scattering calculations of rate coefficients of the $O + H_2 \rightarrow OH + H$ reaction involving both ortho and para hydrogen in the temperature range 100–4000 K. The role of vibrational excitation of H_2 is examined, and it is shown that vibrational excitation of the molecule has a significant effect on reactivity, especially at low temperatures. At 100 K, the rate coefficient increases by about 11 orders of magnitude when the H_2 vibrational quantum number is increased from $v = 0$ to $v = 3$. Initial vibrational state selected cross sections, rate coefficients, and product OH vibrational level distributions are presented for $v = 0$–3 of the H_2 molecule.

Subject headings: astrochemistry — ISM: molecules — molecular data — molecular processes

1. INTRODUCTION

The study of photodissociation regions or photon-dominated regions (PDRs) has attracted considerable attention in recent years, since the first observations of massive star-forming regions (Melnick et al. 1979; Russel et al. 1981). Its importance derives from the fact that far-ultraviolet (FUV) photons penetrate the clouds, heat the gas, and influence the chemical structure, thermal balance, and evolution of the neutral interstellar medium. They also play a significant role in star-forming processes in galaxies (Hollenbach & Tielens 1997). Theoretical models (Tielens & Hollenbach 1985; van Dishoeck & Black 1988; Sternberg et al. 1987; Le Bourlot et al. 1993; Sternberg et al. 1997) of this phenomenon have been developed and used to interpret different events occurring in the neutral interstellar medium. A detailed analysis of the relevant chemical reactions in dense molecular clouds exposed to intense FUV radiation has been given by Sternberg & Dalgarno (1995).

The chemistry in PDRs differs from usual ion-molecular chemical reactions. Because of the FUV flux, photoreactions are very important. Vibrationally excited H_2 (denoted as H_2^*) can play significant role in PDR chemistry. When the gas is hot ($T > 500$ K), the activation energy for reactions of atoms and radicals with H_2 and H_2^* can be overcome, and these reactions dominate. In addition, recombination and charge-transfer reactions can also significantly contribute to the ionization balance.

It has been suggested (Dalgarno 1987; Graf & Dalgarno 1987; Wagner & Graf 1987; Marcus 2004) that the reaction of $O(^3P)$ atoms with vibrationally excited H_2 is the key step in initiating oxygen chemistry in the interstellar medium. Although the $O(^3P) + H_2$ reaction has been the subject of a large number of experimental (Light 1978; Cohen & Westburg 1983; Presser & Gordon 1985; Baulch et al. 1992; Yang et al. 1993; Javoy et al. 2000) and theoretical (Johnson & Winter 1977; Howard et al. 1979; Schinke & Lester 1979; Clary & Connor 1980; Schatz 1985; Joseph et al. 1988; Chatfield et al. 1993; Hoffmann & Schatz 2000) investigations, the studies have largely focused on the ground state of the reagents. The theoretical studies have been mostly based on quasi-classical trajectory (QCT) calculations,

transition state theories, and approximate quantum mechanical methods. Rate coefficients for the reaction involving vibrationally excited H_2 at temperatures of interest in shocked interstellar gases are not available in the literature. Recently, the $O(^3P) + H_2$ reaction has been the topic of renewed interest, due in part to the availability of chemically accurate potential energy surfaces (PESs) of $^3A'$ and $^3A''$ symmetry (Rogers et al. 2000) and new experimental data (Garton et al. 2003) involving crossed molecular beams. Quantum scattering calculations (Garton et al. 2003; Balakrishnan 2004a, 2004b) using the PESs of (Rogers et al. 2000) have been shown to quantitatively reproduce the molecular beam data. The calculations (Balakrishnan 2004a, 2004b) also demonstrated that the J-shifting approximation can be used to compute rate coefficients for the reaction without losing accuracy. Here we report accurate quantum calculations of rate coefficients for

$$O + H_2(v) \rightarrow OH + H \tag{1}$$
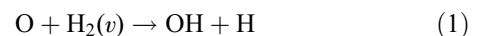
for $v = 0$–3 over the temperature range of 100–4000 K of interest in shock-heated gases.

2. METHOD

The reactive scattering calculations are carried out in hyperspherical coordinates, as implemented in the *ABC* quantum scattering program (Scouteris et al. 2000). The method involves solution of the Schrödinger equation for the motion of the three nuclei on a single Born-Oppenheimer potential energy surface using coupled channel hyperspherical coordinates. Initial-state–selected cross sections corresponding to vibrational-rotational levels (vj) at an incident kinetic energy E_{kin}, are computed using the formula

$$\sigma_{vj}(E_{\mathrm{kin}}) = \sum_{J=0}^{\infty} \sigma_{vj}^J(E_{\mathrm{kin}}), \tag{2}$$

where the partial cross sections for a given value of the total angular momentum quantum number J are given by

$$\sigma_{vj}^J(E_{\mathrm{kin}}) = \frac{\pi}{k_{vj}^2(2j+1)}(2J+1)P_{vj}^J(E_{\mathrm{kin}}). \tag{3}$$
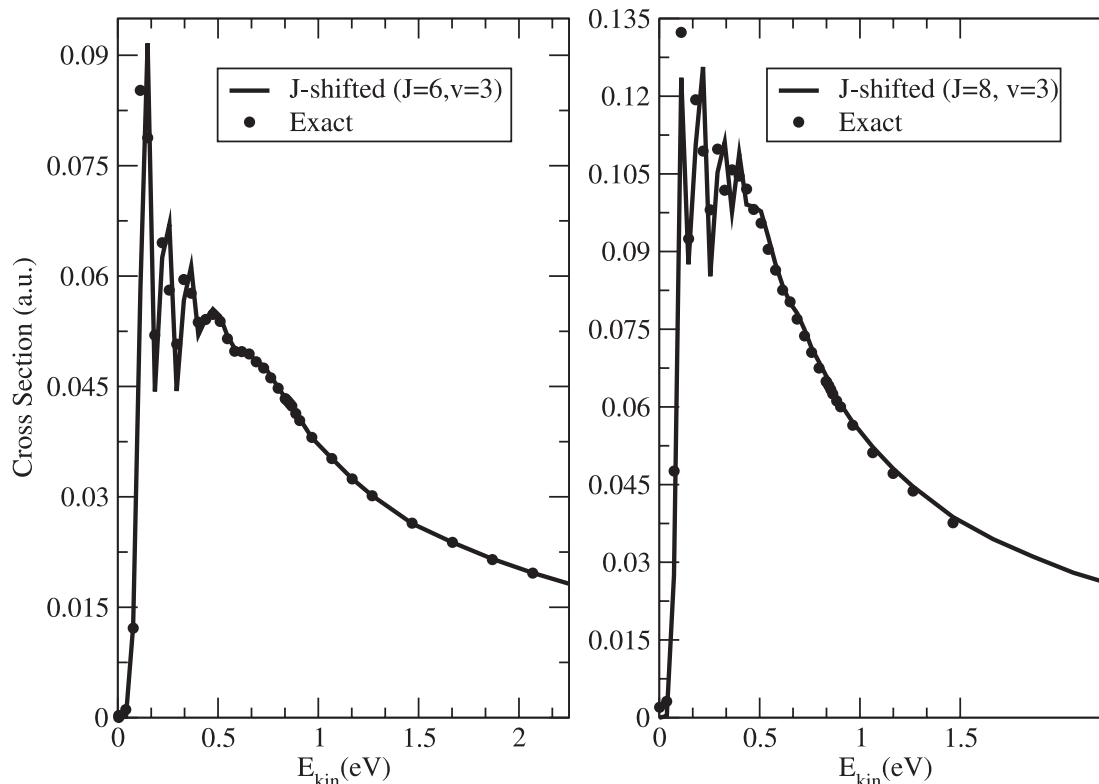
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Fig. 1.—Partial cross sections for $O + H_2(v = 3, j = 0)$ reaction evaluated using exact quantum calculations and the J-shifting approximation. *Left*: Results for $J = 6$ on the $^3A'$ PES. *Right*: Results for $J = 8$ on the $^3A''$ PES.

In equation (3) k_{vj} is the wavevector for the incident channel, and $P_{vj}^J(E_{kin})$ are initial-state–selected reaction probabilities given by

$$P_{vj}^J(E_{kin}) = \sum_{v'j'k'k} |S_{v'j'k',vjk}^J(E_{kin})|^2, \qquad (4)$$

where $S_{v'j'k',vjk}^J(E_{kin})$ is an element of the S-matrix, and the angular momentum projection quantum numbers k and k' are restricted to values $0 \leq k \leq \min(J,j)$ and $0 \leq k' \leq \min(J,j')$.

While quantum calculations of atom-diatom reactions are performed routinely, full calculations that do not employ any decoupling approximations are very time consuming and not practical for higher vibrational levels due to the large number of coupled channels to be included in the solution of the Schrödinger equation. For the $O(^3P) + H_2(v = 0)$ reaction, we have recently reported (Balakrishnan 2004b) explicit quantum calculations of cross sections and rate coefficients for temperatures in the range 200–1000 K. The computed cross sections were found to be in excellent agreement with crossed molecular beam measurement of Garton et al. (2003). We also showed that for the $O(^3P) + H_2(v = 0)$ reaction and its isotopic counterparts (Balakrishnan 2004b; Sultanov & Balakrishnan 2004), accurate results can be obtained using the J-shifting approximation. The basic assumption behind the J-shifting approximation (Bowman 1991) is that the reaction takes place through a transition state and that the rotational energy $E_J^\ddagger$ of the triatomic $[OHH]^\ddagger$ species is not available to overcome the energy barrier of the reaction. The advantage of the J-shifting approximation is that one needs to compute probabilities for only the $J = 0$ case. Cross sections for $J > 0$ are obtained from the $J = 0$ result according to

$$P_{vj}^J(E_{kin}) \approx P_{vj}^{J=0}(E_{kin} - E_J^\ddagger). \qquad (5)$$

The transition state of the OH$_2$ system is linear, and the rotational energy $E_J^\ddagger = B^\ddagger J(J + 1)$, where $B^\ddagger$ is the rotational constant of the transition state complex. The values of the rotational constants are, respectively, 3.127 and 3.154 cm^{-1} for the $^3A'$ and $^3A''$ PESs (Sultanov & Balakrishnan 2004). For our present purpose we employ the J-shifting approximation to compute cross sections and rate coefficients. We also perform full calculations for selected values of J to compare the accuracy of the J-shifting calculations.

Initial-state–selected rate constants are obtained by averaging the corresponding cross sections over a Boltzmann distribution of relative speeds of the colliding partners,

$$k_{vj}(T) = \frac{1}{g} \sqrt{\frac{8k_BT}{\pi\mu}} \int_0^\infty \frac{1}{(k_BT)^2} \sigma_{vj}(E_{kin}) e^{-E_{kin}/k_BT} E_{kin} \, dE_{kin}, \qquad (6)$$

where $g = 3$ is the electronic degeneracy (Schatz et al. 1981), μ is the reduced mass of the atom-molecule system, T is the temperature, and k_B is the Boltzmann constant. The overall rate coefficient is given by the sum of the rate coefficients on the $^3A'$ and $^3A''$ surfaces.

3. RESULTS AND DISCUSSION

We have previously reported rate coefficients of the $O + H_2(v)$ reaction for vibrational levels $v = 0$ and 1 in the temperature range 200–1000 K. In the present study we extend these calculations to compute rate coefficients up to 4000 K and also report new results for $v = 2$ and 3 in the temperature range 100–4000 K. A large number of convergence tests have been carried out to ensure that the results are converged with respect to different parameters that enter into the solution of the Schrödinger equation. Convergence was sought with respect to the maximum
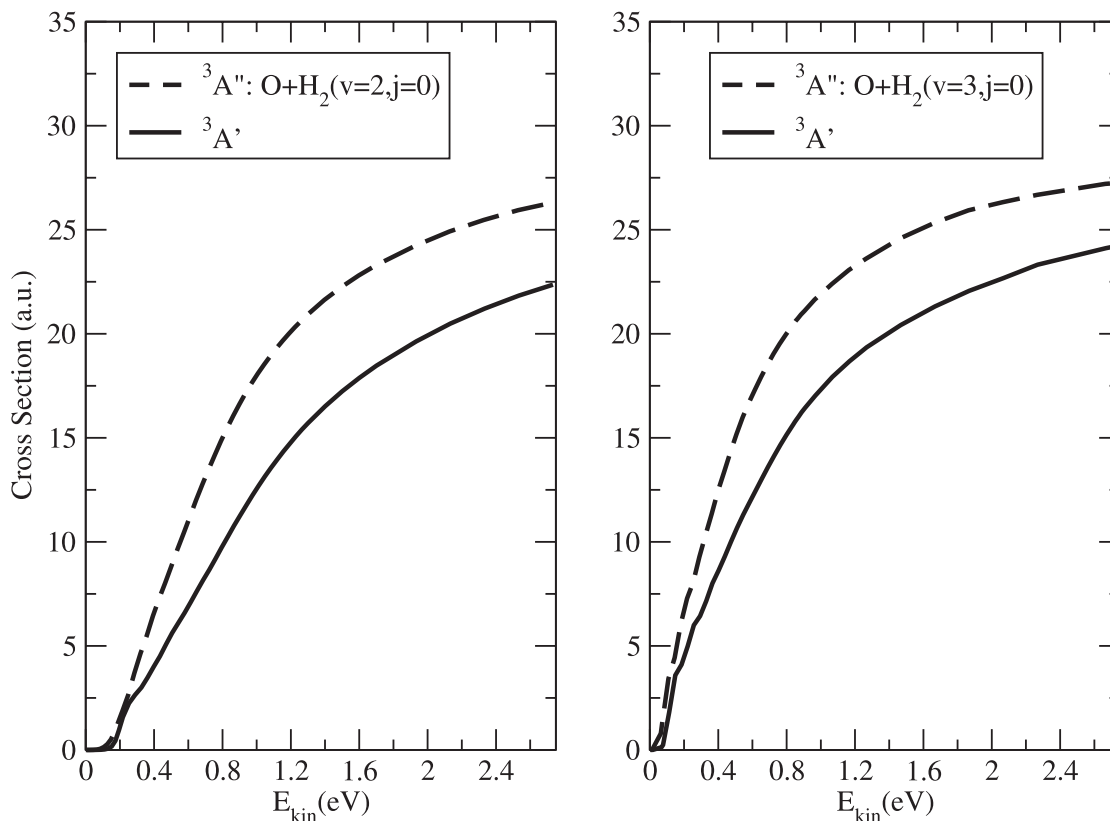
Fig. 2.—Initial vibrational–state selected cross sections for $O + H_2(v, j = 0)$ collisions on the $^3A'$ and $^3A''$ PESs for $v = 2$ (*left*) and $v = 3$ (*right*).

value of the hyperradius, ρ_{max}, at which asymptotic boundary conditions are applied, the cutoff value of the total energy, E_{max}, and the maximum value, j_{max}, of the H_2 and OH rotational levels included in the close-coupled equations. The E_{max} and j_{max} restrict the number of basis functions included in the calculations. Based on extensive convergence tests, we used $\rho_{max} = 25.0a_0$, $\Delta\rho = 0.02a_0$, $E_{max} = 3.8$ eV, and $j_{max} = 36$.

The accuracy of the J-shifting approximation for $v = 0$ and 1 has been demonstrated in our previous studies (Balakrishnan 2004a, 2004b) by comparing with results obtained from exact quantum calculations. Since quantum calculations for all contributing values of J are prohibitively expensive for higher vibrational levels, we restrict our full quantum calculations to partial cross sections, σ_{vj}^J, for $J = 6$ and 8 for $v = 3$. The results are shown in Figure 1 for $O + H_2(v = 3, j = 0)$ reaction on $^3A'$ PES for $J = 6$ and $^3A''$ PES for $J = 8$. It can be seen that for both PESs and J values, the J-shifting approximation does a remarkably good job of reproducing the cross sections, including the oscillatory behavior as a function of the energy. In Figure 2 we show cross sections on both the $^3A'$ and $^3A''$ PESs for $v = 2$ and 3 over an extended range of energy computed using the J-shifting approximation. It is seen that while the $^3A''$ PES makes the major contribution to the reaction, the contribution for the $^3A'$ PES cannot be neglected. The overall cross section is given by the sum of the cross sections computed on the two PESs multiplied by an electronic degeneracy factor of 1/3, i.e., $\sigma_{vj} = \left[\sigma_{vj}(^3A') + \sigma_{vj}(^3A'')\right]/3$. Results shown in Figures 3–7 are evaluated using this expression. Note that the electronic degeneracy factor is included in the expression for the rate coefficient, equation (6).

In Figure 3 we compare the cross sections for $O + H_2(v = 0 - 3, j = 0)$ reactions over a wide range of energy evaluated using the J-shifting approximation. It can be seen that the

threshold of the reaction shifts to lower kinetic energies as the H_2 vibrational level is increased. For $v = 0$ the cross section is essentially zero for incident energies lower than 0.45 eV, showing the presence of a sharp energy threshold. This arises from the energy barrier of about 0.55 eV for the reaction with ground state reagents. The small values of the reaction cross section at energies below the barrier height are due to quantum tunneling. The importance of tunneling in the $O + H_2$ reaction has been discussed in detail in our previous study of the $O + HD/D_2$ reactions (Sultanov & Balakrishnan 2004) and in experimental measurements of the branching ratio between the OH and OD products in the $O + HD$ reaction by Robie et al. (1987). The threshold almost vanishes for $v = 3$ as vibrational energy is
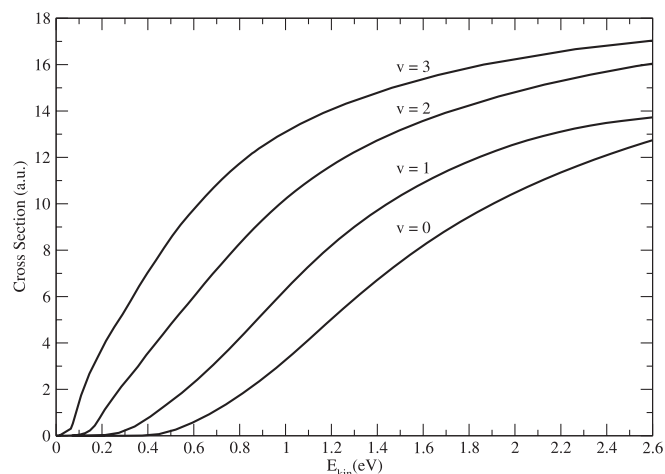

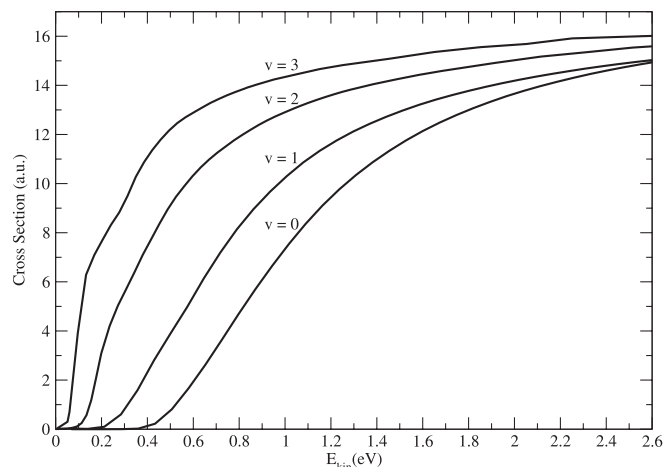Fig. 3.—Initial vibrational state–selected cross sections for $O + H_2(v, j = 0)$ reactions for $v = 0-3$.

Fig. 4.—Initial vibrational state–selected cross sections for $O + H_2(v, j = 1)$ reactions for $v = 0-3$.

Fig. 6.—Vibrationally resolved cross sections for the $O + H_2(v = 2, j = 0) \rightarrow OH(v', j') + H$ reaction, for $v' = 0-2$ (summed over j').

used efficiently to overcome the barrier. The effectiveness of vibrational energy in overcoming energy barriers for endoergic reactions is well known. Similar results for $O + H_2(v = 0 - 3, j = 1)$ reactions are given in Figure 4. It can be seen that rotational excitation of H_2 has a significant effect on reactivity, especially at low energies. The reactivity increases with rotational excitation for all vibrational levels shown in Figure 4. Similar behavior was observed in QCT calculations for $v = 0$ and $v = 1$ by Johnson & Winter (1977). Since the enhancement is more pronounced at low energies, and occurs in both QCT and quantum calculations, we believe that this not a purely quantum effect but a steric effect due to the lowering of the energy barrier as a result of sampling additional regions of the PESs. In general, results are more sensitive to small details of the PESs at low energies.

Product OH vibrational-level–resolved cross sections for $v = 1-3$ of H_2 in $O + p$-H_2 collisions are shown in Figures 5–7. It can be seen that, at low energies, there is a strong correlation between the initial vibrational levels of H_2 and the product OH vibrational levels; the final vibrational level population reflects the initial vibrational excitation. Similar behavior was observed in QCT calculations of Braunstein et al. (2004). At high energies this preference is less prominent, as a number of excited vibrational levels of OH become open. Indeed, for $v = 1$ (see
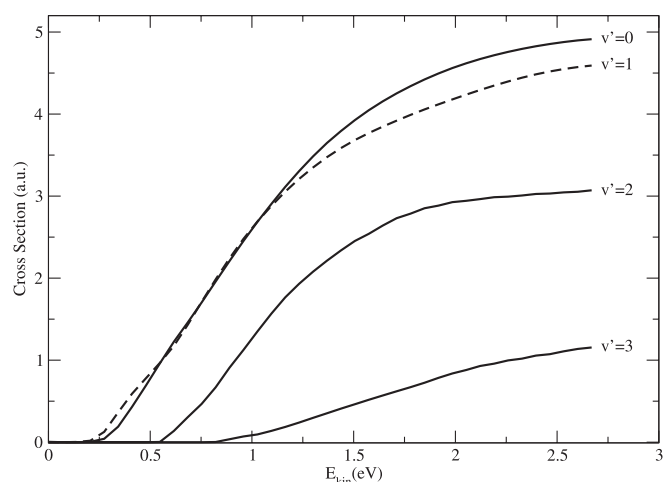
Fig. 5), for kinetic energies above 1.0 eV, the $v' = 0$ level is preferred over the $v' = 1$ level of OH. In Table 1 we compare OH vibrational-level–resolved cross sections from our calculations with the QCT results of Braunstein et al. (2004) for selected values of collision energies for the $O + p$-$H_2(v = 3)$ reaction. It can be seen that the quantum and QCT results predict similar population distribution of OH vibrational levels, but the QCT calculations overestimates the results by about 20%–30%.

Rate coefficients of the $O + H_2(v)$ reaction for $v = 0-3$ for both ortho and para H_2 are given in Table 2 for temperatures of 100–4000 K. Results for $v = 0$ from 200–1000 K and $v = 1$ from 150–1000 K for p-H_2 have been reported in our previous publications (Balakrishnan 2004a, 2004b), but we reproduce them here for completeness. It can be seen from these results that at 100 K, vibrational excitation of H_2 from $v = 0$ to $v = 3$ increases the rate coefficient by about 11 orders of magnitude. The effect of vibrational excitation is largest at the lowest temperatures, as vibrational energy is used efficiently to overcome the energy barrier. For example, at 500 K, 3 quanta vibrational excitation of H_2 increases the rate coefficient by about 4 orders of magnitude, while at 3000 K the increase is only about a factor of 10.

Fig. 5.—Vibrationally resolved cross sections for the $O + H_2(v = 1, j = 0) \rightarrow OH(v', j') + H$ reaction, for $v' = 0$ and 1 (summed over j').

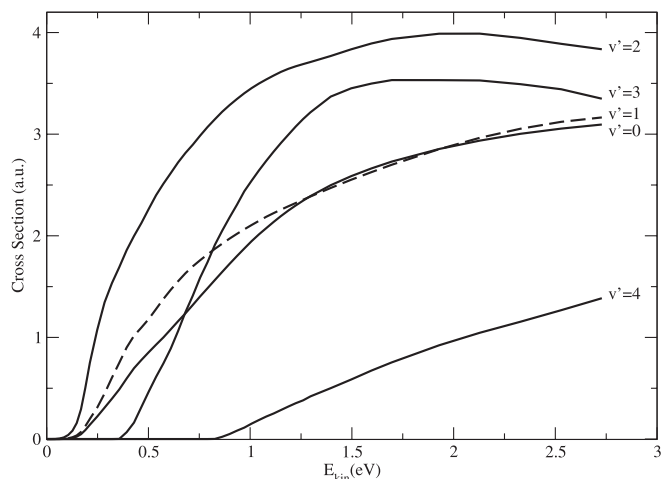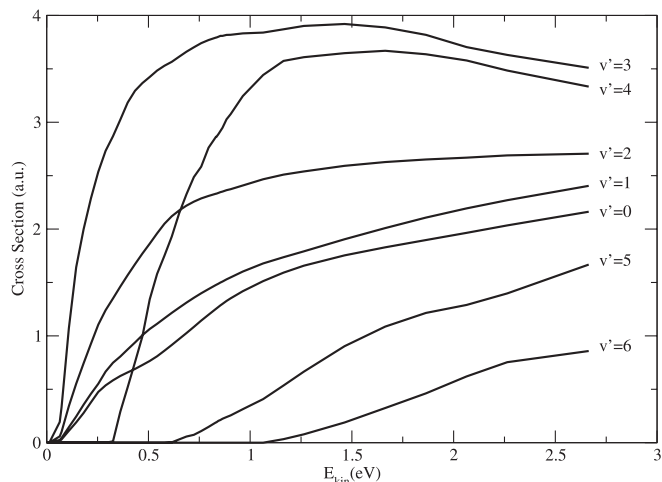Fig. 7.—Vibrationally resolved cross sections for the $O + H_2(v = 3, j = 0) \rightarrow OH(v', j') + H$ reaction, for $v' = 0-3$ (summed over j').

TABLE 1
VIBRATIONALLY RESOLVED CROSS SECTIONS (SUMMED OVER j') IN a.u. FOR $O(^3P) + H_2(v = 3, j = 0) \rightarrow OH(v') + H$ REACTION FOR SPECIFIC VALUES OF COLLISION ENERGY FROM THIS WORK AND THE QCT RESULTS FROM TABLE 1 OF BRAUNSTEIN ET AL. (2004)

E_{kin} (kcal mol^{-1})	THIS WORK				QCT			
	$v' = 0$	$v' = 1$	$v' = 2$	$v' = 3$	$v' = 0$	$v' = 1$	$v' = 2$	$v' = 3$
10.00......................................	0.69	0.94	1.67	3.29	0.69	1.29	2.59	3.94
18.00......................................	1.18	1.42	2.30	3.76	1.32	2.15	2.85	4.53
26.00......................................	1.57	1.72	2.50	3.86	1.69	2.49	3.45	4.49

TABLE 2
RATE CONSTANTS (cm^3 molecule^{-1} s^{-1}) FOR $O + H_2(v, j)$ REACTION FOR $v = 0-3$ OF PARA AND ORTHO H_2

T (K)	PARA-H_2				ORTHO-H_2			
	$v = 0$	$v = 1$	$v = 2$	$v = 3$	$v = 0$	$v = 1$	$v = 2$	$v = 3$
100...............	5.94E−25	3.38E−18	1.83E−15	5.36E−14	6.77E−24	9.89E−17	5.88E−15	1.82E−13
150...............	2.28E−22	3.59E−17	6.21E−15	2.23E−13	1.43E−21	1.75E−16	1.66E−14	6.56E−13
200...............	1.05E−20	2.00E−16	2.05E−14	6.10E−13	5.97E−20	4.24E−16	6.06E−14	1.74E−12
250...............	2.08E−19	8.09E−16	5.62E−14	1.25E−12	1.15E−18	1.42E−15	1.80E−13	3.51E−12
300...............	2.27E−18	2.64E−15	1.28E−13	2.14E−12	1.19E−17	4.74E−15	4.22E−13	5.86E−12
350...............	1.54E−17	7.15E−15	2.52E−13	3.25E−12	7.59E−17	1.36E−14	8.29E−13	8.65E−12
400...............	7.25E−17	1.65E−14	4.39E−13	4.55E−12	3.36E−16	3.28E−14	1.42E−12	1.18E−11
500...............	7.40E−16	6.15E−14	1.04E−12	7.57E−12	3.13E−15	1.29E−13	3.21E−12	1.86E−11
600...............	3.88E−15	1.63E−13	1.95E−12	1.10E−11	1.54E−14	3.50E−13	5.75E−12	2.57E−11
700...............	1.35E−14	3.45E−13	3.18E−12	1.48E−11	5.05E−14	7.45E−13	8.93E−12	3.30E−11
800...............	3.58E−14	6.28E−13	4.70E−12	1.89E−11	1.28E−13	1.35E−12	1.26E−11	4.03E−11
900...............	7.85E−14	1.03E−12	6.50E−12	2.31E−11	2.70E−13	2.19E−12	1.68E−11	4.75E−11
1000.............	1.50E−13	1.55E−12	8.54E−12	2.75E−11	4.99E−13	3.27E−12	2.12E−11	5.47E−11
1200.............	4.17E−13	3.00E−12	1.33E−11	3.67E−11	1.30E−12	6.15E−12	3.09E−11	6.87E−11
1400.............	9.03E−13	5.00E−12	1.87E−11	4.63E−11	2.66E−12	9.94E−12	4.12E−11	8.23E−11
1600.............	1.66E−12	7.55E−12	2.48E−11	5.62E−11	4.66E−12	1.45E−11	5.18E−11	9.56E−11
1800.............	2.73E−12	1.06E−11	3.14E−11	6.63E−11	7.32E−12	1.98E−11	6.27E−11	1.08E−10
2000.............	4.14E−12	1.42E−11	3.84E−11	7.65E−11	1.06E−11	2.57E−11	7.35E−11	1.21E−10
2200.............	5.90E−12	1.83E−11	4.58E−11	8.68E−11	1.45E−11	3.20E−11	8.44E−11	1.33E−10
2400.............	8.01E−12	2.27E−11	5.35E−11	9.71E−11	1.90E−11	3.87E−11	9.51E−11	1.44E−10
2600.............	1.05E−11	2.76E−11	6.13E−11	1.07E−10	2.40E−11	4.58E−11	1.06E−10	1.56E−10
2800.............	1.33E−11	3.28E−11	6.94E−11	1.18E−10	2.95E−11	5.31E−11	1.16E−10	1.66E−10
3000.............	1.64E−11	3.83E−11	7.76E−11	1.28E−10	3.54E−11	6.06E−11	1.27E−10	1.77E−10
3300.............	2.17E−11	4.71E−11	9.00E−11	1.43E−10	4.48E−11	7.21E−11	1.42E−10	1.92E−10
4000.............	3.63E−11	6.92E−11	1.19E−10	1.77E−10	6.90E−11	9.94E−11	1.75E−10	2.26E−10

TABLE 3
RATE COEFFICIENTS FOR THE O + H$_2(v = 2)$ REACTION

T (K)	$k^t_{v=2}(T)$	$k^s_{v=2}(T)$
100........................	2.17E−15	4.87E−15
150........................	1.43E−14	1.40E−14
200........................	6.64E−14	5.06E−14
250........................	2.14E−13	1.49E−13
300........................	5.17E−13	3.49E−13
350........................	1.02E−12	6.84E−13
400........................	1.73E−12	1.18E−12
500........................	3.78E−12	2.67E−12
600........................	6.59E−12	4.80E−12
700........................	1.01E−11	7.49E−12
800........................	1.41E−11	1.07E−11
900........................	1.86E−11	1.42E−11
1000........................	2.36E−11	1.81E−11
1200........................	3.45E−11	2.65E−11
1400........................	4.64E−11	3.56E−11
1600........................	5.90E−11	4.51E−11
1800........................	7.19E−11	5.48E−11
2000........................	8.50E−11	6.48E−11
2200........................	9.82E−11	7.47E−11
2400........................	1.11E−10	8.47E−11
2600........................	1.25E−10	9.47E−11
2800........................	1.38E−10	1.05E−10
3000........................	1.51E−10	1.14E−10
3300........................	1.69E−10	1.29E−10
4000........................	2.11E−10	1.61E−10

NOTE.—In cm^3 molecule^{-1} s^{-1}; assuming thermal $[k^t_{v=2}(T)]$ and statistical $[k^s_{v=2}(T)]$ equilibrium between ortho and para H$_2$.

From the rate coefficients in Table 2 for ortho and para H$_2$ one could compute rate coefficients for O + H$_2(v = 0 - 3)$ collisions assuming a statistical equilibrium of ortho and para H$_2$:$k^s_v(T) = \frac{1}{4}k^{para}_v(T) + \frac{3}{4}k^{ortho}_v(T)$. However, if ortho and para H$_2$ exist in thermal equilibrium, the overall rate coefficient is given by

$$k^t_v(T) = \frac{\sum_{j=0,2,4,..} Q_j k^{para}_{vj}(T) + 3\sum_{j=1,3,5,..} Q_j k^{ortho}_{vj}(T)}{Q_{para} + 3Q_{ortho}}, \quad (7)$$

where $Q_j = (2j + 1)e^{-E_j/k_B T}$, and $Q_{para} = \Sigma_{j=0,2,4,..} Q_j$ and $Q_{ortho} = \Sigma_{j=1,3,5,..} Q_j$ are the rotational partition functions of para and ortho H$_2$, respectively. Rotational levels of H$_2$ up to 14 for para-H$_2$ and 15 for ortho-H$_2$ have been included in the summations above in evaluating the rate coefficients. Rate coefficients for the O + H$_2$ reaction evaluated assuming thermal or statistical equilibrium are given in Table 3 for the $v = 2$ level of H$_2$. It can be seen that except at the lowest temperature of 100 K, the assumption of thermal equilibrium leads to rate coefficients that are larger by about 10%–40%. We believe that the cross sections and rate coefficients reported here will form important components of quantitative models of oxygen chemistry in PDRs.

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