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COLLISIONAL RATES FOR VIBRATIONAL-ROTATIONAL TRANSITIONS IN CIRCUMSTELLAR SiO MASERS[1]

RONALD J. BIENIEK
Department of Physics, University of Missouri-Rolla

AND

SHELDON GREEN
NASA Goddard Space Flight Center, Institute for Space Studies
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ABSTRACT

Calculations for rotational population inversion in circumstellar SiO masers require collisional rates for vibrational-rotational transitions. This *Letter* reports quantum mechanical, state-to-state collisional rate coefficients for pure rotational and vibrational-rotational transitions among the first three vibrational states of SiO. These are expressed in terms of simple two-parameter power-law fits accurate in the temperature range 1000–3000 K.

Subject headings: masers—molecular processes

I. INTRODUCTION

The explanation of the pumping mechanism for circumstellar SiO masers has proved elusive. Masering emission has been observed between low-lying rotational levels of the first three excited vibrational states of SiO in close proximity to, and probably in the outer atmospheres of, certain late-type stars (Snyder and Buhl 1974; Buhl *et al.* 1974; Scalise and Lepine 1978; see Reid and Moran 1981 for a current tabulation). Two possible sources of weak maser emission in the ground vibrational state have also been reported (Buhl *et al.* 1975; Dickinson *et al.* 1978). Interferometric observations by Moran *et al.* (1979) and Lane *et al.* (1980) confirm that masering in different vibrational states can occur in the same region. Devising a model in which so many different vibrational states can participate in masering has proved difficult. Various optical mechanisms (Geballe and Townes 1974; Kwan and Scoville 1974; Deguchi and Iguchi 1976; Robinson and Van Blerkom 1981) and collisional pumping schemes (Elitzur 1980; Watson, Elitzur, and Bieniek 1980; Bujarrabal and Nguyen-Q.-Rieu 1981) have been proposed.

To model properly the populations of the masering levels requires state-to-state rate coefficients for vibrational-rotational transitions in SiO induced by collisions with H_2, but these have not been available. Bujarrabal and Nguyen-Q.-Rieu (1981) have used state-to-state rates inferred from CO data but found that uncertainties in the rates strongly affected their results. In a recent article, Robinson and Van Blerkom (1981, p. 568) declare, "Unfortunately, even approximate collisional rates for SiO at the relatively high temperature of a stellar envelope do not exist, and it is unlikely that they can be either calculated or measured in the near future." Nonetheless, we report such coefficients in this *Letter*, based on quantum mechanical cross sections. The parameters presented allow one to determine state-to-state rates $k_{v_i, j_i \to v_f, j_f}(T)$ for $v_{i,f} = 0$, 1, 2 and $|j_i - j_f| \lesssim 39$, where the v's and j's are vibrational and rotational quantum numbers of SiO.

II. QUANTAL CALCULATIONS

Because of the near sphericity of H_2 and its large rotational-vibrational spacing, one can treat H_2 approximately as a structureless collisional partner with the electronic properties of He (Green 1977; Green *et al.* 1978). An approximate electron-gas He-SiO potential hypersurface, reported elsewhere (Bieniek and Green 1981), was employed in the present calculations to describe the interaction between SiO and structureless H_2. To obtain thermal rate coefficients appropriate for masering stellar environments, state-to-state cross sections, $\sigma_{v_i, j_i \to v_f, j_f}(E_c)$, were computed at five collisional energies $E_c = 0.129$ (0.065) 0.389 eV, i.e., $\frac{3}{2}kT$ for $T = 1000$ (500) 3000 K. These were then integrated over Boltzmann distributions of collisional energies. Because the rotational energy spacings are small compared with these

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collisional energies, we employed the infinite-order sudden (IOS) approximation in which the rotational levels of SiO are treated as degenerate (see Parker and Pack 1978). Within this approximation, the state-to-state rate coefficients for arbitrary j_i and j_f can be obtained from the rates into the $j' = 0$ level (Smith and Pritchard 1981):

$$k^{\mathrm{IOS}}_{v_i, j_i \to v_f, j_f}(T) = g_{j_f} \exp\left[(\varepsilon_i - \varepsilon^*)/kT\right] \sum_{j=|j_i - j_f|}^{j=j_i+j_f} \begin{pmatrix} j_i & j_f & j \\ 0 & 0 & 0 \end{pmatrix}^2 g_j k^{\mathrm{IOS}}_{v_u, j \to v_l, 0}(T), \tag{1}$$

where (:::) is a 3-j symbol; $g_j = (2j + 1)$; v_u is the greater of v_i and v_f, while v_l is the lesser; ε_s is the vibrational-rotational energy of SiO in state s; and ε^* is the greater of ε_i and ε_f.

The problem then reduces to the computation of the $\sigma_{v_u, j \to v_l, 0}$ cross sections and integration over a Boltzmann distribution of collisional energies to obtain thermal rates. The calculation of cross sections at the five energies used a quantal adiabatic, distorted-wave technique (Eno and Balint-Kurti 1979; Bieniek 1980). Vibrational S-matrices for $v_u = 0, 1, 2$ and $\Delta v = 0, -1$ were computed at 48 orientational angles to ensure accuracy of the rotational cross sections up to at least $j = 39$. The accuracy of the adiabatic, distorted-wave approach has been difficult to establish because of the general paucity of accurate numerical rotational-vibrational cross sections. In this study, we numerically compared this method at $E_c = 0.323$ eV with a standard two-state coupled-equations technique (Green 1979). For pure rotational cross sections, the two methods generally agreed to within 5%; for vibrational-rotational cross sections, agreement was typically within 15%. Total rates disagreed by only a few percent. These results indicate that the faster adiabatic distorted-wave method is sufficiently accurate.

III. TOTAL RATES

It is sometimes convenient to consider total rates that have been summed over final rotational levels. In the IOS approximation, total cross sections are independent of the initial rotational level. The total cross section for inelastic, pure rotational excitation is

$$\sigma_r^v(E_c) = \sum_{j' \neq 0} \sigma^{\mathrm{IOS}}_{v,0 \to v,j'}(E_c) = \sum_{j \neq 0} g_j \sigma^{\mathrm{IOS}}_{v,j \to v,0}(E_c), \tag{2}$$

and the total cross section for vibrational de-excitation is

$$\sigma_{v \to v-1}(E_c) = \sum_{j'} \sigma^{\mathrm{IOS}}_{v,0 \to v-1,j'}(E_c) = \sum_{j} g_j \sigma^{\mathrm{IOS}}_{v,j \to v-1,0}(E_c) \tag{3}$$

with analogous definitions for the total rates $k_r^v(T)$ and $k_{v \to v-1}(T)$.

It was reported earlier (Bieniek and Green 1981) that $\sigma_r^{v=1}(E_c)$ is independent of E_c, while $\sigma_{v=1 \to 0}(E_c)$ obeys a power law of $(E_c)^{2.2}$. A more refined analysis confirms the power-law behavior but yields slightly different values for the exponents. Putting the total cross sections in the form $\sigma(E_c) = \sigma(E_0)(E/E_0)^p$, with $E_0 = 0.259$ eV, we find (in cm^2)

$$\sigma_r^{v=0}(E_c) = 2.80 \times 10^{-15} \left(\frac{E_c}{E_0}\right)^{-0.11}, \tag{4}$$

$$\sigma_r^{v=1}(E_c) = 2.96 \times 10^{-15} \left(\frac{E_c}{E_0}\right)^{-0.11}, \tag{5}$$

$$\sigma_r^{v=2}(E_c) = 3.16 \times 10^{-15} \left(\frac{E_c}{E_0}\right)^{-0.18}, \tag{6}$$

$$\sigma_{v=1 \to 0}(E_c) = 3.48 \times 10^{-18} \left(\frac{E_c}{E_0}\right)^{2.13}, \tag{7}$$

$$\sigma_{v=2 \to 1}(E_c) = 1.83 \times 10^{-17} \left(\frac{E_c}{E_0}\right)^{2.39}. \tag{8}$$

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The total rates for inelastic pure rotational excitation are then (in $cm^3\ s^{-1}$)

$$k_r^{v=0}(T) = 1.31 \times 10^{-9}\left(\frac{T}{T_0}\right)^{0.39}, \tag{9}$$

$$k_r^{v=1}(T) = 1.39 \times 10^{-9}\left(\frac{T}{T_0}\right)^{0.39}, \tag{10}$$

$$k_r^{v=2}(T) = 1.49 \times 10^{-9}\left(\frac{T}{T_0}\right)^{0.32}, \tag{11}$$

where $T_0 = 2000$ K. These are adequately described by the single equation

$$k_r^{v}(T) = (1.31 + 0.09v) \times 10^{-9}\left(\frac{T}{T_0}\right)^{0.36}. \tag{12}$$

The total rates for vibrational de-excitation are

$$K_{v=1\to 0}(T) = 4.85 \times 10^{-12}\left(\frac{T}{T_0}\right)^{2.63}, \tag{13}$$

$$K_{v=2\to 1}(T) = 3.25 \times 10^{-11}\left(\frac{T}{T_0}\right)^{2.89}. \tag{14}$$

Anharmonic effects produce the nearly order-of-magnitude difference between these last two rates, since they would differ by only a factor of 2 in a purely harmonic target.

IV. STATE-TO-STATE RATES

In order to facilitate the averaging over collisional energies needed for state-to-state thermal rate coefficients, the energy dependence of the $\sigma_{v_u, j\to v_l, 0}$ was fitted to a function of the form $AE_c^{\alpha}\exp(aE_c) + B$. This form was chosen because spurious undulations would be minimized, and the thermal average could be evaluated analytically. In some cases problems arose outside the energy interval [0.129 eV, 0.389 eV]; the $\exp(aE_c)$ factor often generated a spuriously large contribution at large E_c, while the sum could be negative at low energies. To solve this, we assumed that the state-to-state cross sections outside this energy interval had the same energy dependence as the corresponding total cross sections to which they contribute. Thus,

$$\sigma_{v_u, j\to v_l, 0}(E_c) = \begin{cases} \sigma_{v_u, j\to v_l, 0}(E_{mn})\left(\dfrac{E_c}{E_{mn}}\right)^p & \text{for } E < E_{mn}, \\ AE_c^{\alpha}e^{aE_c} + B & \text{for } E_{mn} \leqslant E \leqslant E_{mx}, \\ \sigma_{v_u, j\to v_l, 0}(E_{mx})\left(\dfrac{E_c}{E_{mx}}\right)^p & \text{for } E_{mx} < E, \end{cases} \tag{15}$$

where $E_{mn} = 0.129$ eV and $E_{mx} = 0.389$ eV, and p is the appropriate power from among equations (4)–(8). Using equation (15), the integral over collisional energies can be evaluated analytically in terms of incomplete gamma functions.

Despite the complexity of the fitting function used for cross sections, numerical values of rate coefficients in the relevant temperature range of 1000 K $\leqslant T \leqslant$ 3000 K were found to be accurately described by a simple, two-parameter power law:

$$k_{v_u, j\to v_l, 0}(T) = k_{v_u, j\to v_l, 0}(T_0)\left(\frac{T}{T_0}\right)^{q(j, v_u, v_l)}, \tag{16}$$

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TABLE 1

PARAMETERS FOR RATE COEFFICIENTS IN THE FORM $g_j k_{v_u, j \to v_l, 0}(T) = g_j k_{v_u, j \to v_l, 0}(T_0)(T/T_0)^{q(j, v_u, v_l)}$ FOR $T_0 = 2000$ K[a]

	PARAMETERS									
	$v_u = 0, v_l = 0$		$v_u = 1, v_l = 1$		$v_u = 2, v_l = 2$		$v_u = 1, v_l = 0$		$v_u = 2, v_l = 1$	
j	$g_j k_{0, j \to 0, 0}(T_0)$[b]	q	$g_j k_{1, j \to 1, 0}(T_0)$[b]	q	$g_j k_{2, j \to 2, 0}(T_0)$[b]	q	$g_j k_{1, j \to 0, 0}(T_0)$[b]	q	$g_j k_{2, j \to 1, 0}(T_0)$[b]	q
0	280.00	0.07	240.00	0.21	312.00	0.17	0.33	2.65	7.52	2.83
1	2.91	0.17	4.31	0.07	8.30	0.00	0.27	2.39	1.08	2.93
2	28.20	0.31	33.00	0.22	35.40	0.16	0.87	2.46	9.20	2.81
3	2.71	0.30	2.96	0.22	3.80	0.08	0.68	2.42	3.55	2.86
4	15.10	0.33	17.10	0.23	16.70	0.18	1.49	2.43	8.07	2.72
5	3.34	0.31	3.26	0.33	3.27	0.24	1.05	2.34	6.65	2.82
6	11.90	0.31	13.40	0.26	13.70	0.19	2.03	2.35	6.81	2.60
7	4.21	0.31	4.07	0.37	3.52	0.34	1.45	2.35	8.82	2.70
8	9.26	0.32	10.00	0.33	10.80	0.22	2.69	2.41	6.25	2.47
9	4.81	0.33	4.68	0.41	3.59	0.47	1.66	2.48	11.00	2.73
10	7.21	0.33	7.30	0.39	8.07	0.24	2.85	2.47	6.46	2.50
11	4.81	0.37	4.57	0.46	3.46	0.55	1.81	2.59	10.70	2.67
12	5.09	0.41	4.98	0.53	6.03	0.36	2.87	2.52	8.30	2.68
13	4.88	0.38	4.60	0.44	3.48	0.49	1.67	2.55	9.85	2.69
14	3.00	0.62	2.91	0.78	3.86	0.56	3.11	2.68	10.60	2.83
15	4.60	0.37	4.21	0.48	3.48	0.44	1.80	2.67	8.51	2.71
16	1.96	0.81	1.32	1.00	2.36	0.80	2.78	2.82	13.70	2.98
17	4.05	0.38	3.42	0.61	3.06	0.40	1.67	2.54	7.19	2.73
18	1.56	0.70	0.76	1.15	1.53	1.05	1.87	2.81	12.60	3.05
19	3.69	0.37	2.68	0.81	2.40	0.48	1.20	2.36	5.05	2.51
20	0.75	0.86	0.56	1.10	1.13	1.24	1.51	2.88	11.00	3.01
21	3.22	0.37	2.03	1.11	1.87	0.75	1.27	2.43	3.92	2.26
22	0.57	0.87	0.43	0.80	0.91	1.13	1.15	2.97	11.60	3.06
23	2.46	0.48	1.52	1.41	1.48	1.11	1.32	2.59	5.69	2.60
24	0.53	0.74	0.43	0.77	0.72	0.98	0.67	2.85	7.87	3.60
25	1.68	0.77	1.07	1.64	1.19	1.43	1.43	2.81	8.53	2.93
26	0.56	0.50	0.39	0.99	0.65	0.97	0.58	2.83	4.97	2.79
27	1.05	1.26	0.66	1.78	0.85	1.62	1.29	2.99	11.10	3.14
28	0.60	0.41	0.34	1.20	0.45	1.15	0.47	2.87	3.87	2.76
29	0.60	1.71	0.38	1.84	0.51	1.57	0.83	3.06	7.99	3.07
30	0.53	0.50	0.31	1.45	0.26	1.13	0.34	2.74	2.70	2.62
31	0.37	1.96	0.22	1.86	0.41	1.61	0.58	3.16	5.61	2.96
32	0.37	0.85	0.26	1.72	0.19	1.30	0.32	2.82	3.28	2.80
33	0.26	1.79	0.12	1.75	0.34	1.66	0.33	3.19	5.39	3.05
34	0.24	1.38	0.19	1.95	0.14	1.47	0.31	3.00	3.92	2.95
35	0.21	1.57	0.08	1.64	0.23	1.68	0.20	3.12	4.84	3.04
36	0.18	2.03	0.11	2.04	0.12	1.68	0.31	3.19	3.85	3.09
37	0.18	1.45	0.07	1.65	0.15	1.60	0.11	2.94	6.64	3.14
38	0.11	2.21	0.05	2.01	0.08	1.76	0.13	3.21	2.29	3.08
39	0.14	1.72	0.06	1.81	0.12	1.65	0.10	3.00	7.66	3.24

[a] $g_j = (2j + 1)$.
[b] In units of 10^{-11} cm^3 s^{-1}.

where $T_0 = 2000$ K. Values of $k_{v_u, j \to v_l, 0}(T_0)$ and $q(j, v_u, v_l)$ for $v_u = 0, 1, 2, \Delta v = 0, -1$, and $0 \leqslant j \leqslant 39$ are displayed in Table 1, which is the primary result of this *Letter*. Note that, for low j, the rates for even j are larger than for odd j, reflecting a "near homonuclear propensity."

It is informative to compare our state-to-state rates for pure-rotational de-excitation with those used by Robinson and Van Blerkom (1981) in their analysis of ground vibrational state masering. For low-lying rotational states ($j \lesssim 20$), their rates are given by

$$k^{RvB}_{0, j \to 0, 0}(T) = 6.4 \times 10^{-12} \left(\frac{T}{2000 \text{ K}} \right)^{-1/2} g_j^{-1} \left(1 + \frac{j}{1 + (j - 2)^2} \right). \tag{17}$$

They do not account for the even-j–odd-j oscillation of the rates that we observe. Furthermore, their temperature

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dependence of $T^{-0.5}$ can be compared with our prediction of approximately $T^{+0.4}$. This difference arises from their utilization of a heuristic expression given by Goldreich and Kwan (1974) that significantly overestimates the contributions of high j to total rates. On the average, their pure rotational inelastic rates are about an order of magnitude smaller than ours.

It is somewhat difficult to judge the absolute accuracy of our calculated rates owing to a paucity of experimental data and theoretical studies for this or related systems. The major source of error is undoubtedly the assumed interaction potential; the molecular scattering approximations and the various numerical methods have been tested and found to be accurate to better than about 25% for individual rate coefficients. For pure rotational excitation, extensive experience with the CO-He system suggests that the electron gas potential used here may give errors of up to a factor of 2 for individual rates, but that total rates—which reflect mainly the geometric size of SiO—are unlikely to be wrong by more than 10% (Green and Thomas 1980, and references therein). Verter and Rabitz (1976) have compared experimental with theoretical vibrational rates for CO-He using an electron gas potential analogous to that employed here, but that work suffers from less rigorous scattering approximations and difficulties in interpreting the experimental data. Nonetheless, they find agreement for total vibrational rates within about a factor of 3 at room temperature and perhaps slightly worse at elevated temperatures. Based on this and other studies, we believe that our total vibrational rates are unlikely to be in error by more than an order of magnitude. The typical error for the type of calculation reported here may well be lower than this conservative limit, but not enough comparative studies are available to warrant a more definitive estimate. Some further caution must be voiced concerning our assumption that the electronic interaction of H_2 can be approximated by that of He. This approximation is rigorous at low temperatures where H_2 is in its lowest $j = 0$ level; in higher rotational levels, however, the H_2 quadrupole has a significant interaction at long range with the SiO dipole moment and dipole derivative. This probably enhances dipole allowed rates ($\Delta j = \pm 1$) by a factor of 2–3. Further study of this point is warranted. Nonetheless, the detailed rates presented here should be useful in modeling SiO masers and choosing among the various collisional and optical pumping schemes.

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RONALD J. BIENIEK: Department of Physics, University of Missouri-Rolla, 102 Physics Building, Rolla, MO 65401

SHELDON GREEN: NASA Goddard Space Flight Center, Institute for Space Studies, 2880 Broadway, New York, NY 10025

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