QUANTUM-MECHANICAL STUDY OF ROTATIONAL AND VIBRATIONAL TRANSITIONS IN CO INDUCED BY H ATOMS

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ABSTRACT

We report rate coefficients for rotational and vibrational transitions in CO induced by H atoms using quantum-mechanical scattering calculations and the H-CO interaction potential of Keller et al. We use the infinite-order sudden approximation for vibrational transitions and the close-coupling method for rotational transitions. Rate coefficients are presented for temperatures $5 \text{ K} < T < 3000 \text{ K}$. Differences of a factor of 30 are found for rate coefficients for low temperatures below 100 K compared to earlier results of Green and Thaddeus. The discrepancies are attributed to the differences in the details of the interaction potentials, especially the long-range part to which the low-temperature rate coefficients are most sensitive. There is good spectroscopic evidence that the potential-energy surface employed here reproduces the resonance energies and widths of the HCO system better than any previously available HCO interaction potentials.

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

On-line material: machine-readable table

1. INTRODUCTION

Excitation of rotational and vibrational levels of carbon monoxide occurs in a wide variety of astrophysical environments. Emissions from levels with rotational quantum numbers j up to 30 have been seen from shocked regions of the interstellar gas and from photon-dominated or photodissociation regions (Watson et al. 1985; Liu et al. 1996; Cernicharo et al. 1996; Cox et al. 1996; Nisini et al. 1996). They make a major contribution to the cooling of these objects, and they provide a powerful diagnostic probe of the physical conditions in which the emissions take place. Emissions from and absorptions into vibrationally excited levels play a similar role in studies of the atmospheres and envelopes of stars (Hinkle & Lambert 1975; Carbon, Milkey, & Heasley 1976; Sahai & Wannier 1985; Ayres & Wiedemann 1989; Wiedemann et al. 1994; Ryde et al. 1999; Yan et al. 1999; Uitenbroek 2000), the Becklin-Neugebauer object (Scoville, Krotkov, & Wang 1980), and the ejecta of supernova 1987A (Liu, Dalgarno, & Lepp 1992; Liu & Dalgarno 1995; Yan & Dalgarno 1998). Departures from local thermodynamic equilibrium occur, and the interpretations of the observations are sensitive to the excitation rate coefficients for collisions of CO with H, H₂, and He.

Quantum calculations of the rotational excitation rate coefficients for H-CO collisions have been carried out by Chu & Dalgarno (1975) and Green & Thaddeus (1976) using semiempirical potential-energy surfaces. The results of Green & Thaddeus have been widely adopted for astrophysical applications (Waring, Benayoun, & Viala 1996). Estimates of vibrational quenching rate coefficients for H-CO collisions have been made by Scoville et al. (1980) based on the measurements of von Rosenberg, Taylor, & Teare (1971) and by Ayres & Wiedemann (1989) based on the measurements of Glass & Kironde (1982). Much improved potential-energy surfaces have been constructed by Bowman, Bittman, & Harding (1986) and by Keller et al. (1996) and have been tested by experiments (Murray et al. 1986; Ni, Flynn, & Green 1994; Tobiason, Dunlop, & Rohlfing 1995). Calculations based on the two potentials of inelastic

scattering at specific energies have been reported (Lee & Bowman 1987; Chawla et al. 1988; Gazdy, Bowman, & Sun 1988; Ni et al. 1994; Green, Pan, & Bowman 1995; Qi & Bowman 1996) that generally confirm the accuracy of the two surfaces but also demonstrate the sensitivity of the rate coefficients to the details of the surfaces.

We adopt the surface of Keller et al. (1996) based on the ab initio calculation of Werner et al. (1995) to calculate rotational and vibrational transition rate coefficients over a range of astrophysically relevant temperatures. Spectroscopic studies of resonance energies and widths of the HCO system have shown that this surface reproduces the measurements better than the surface of Bowman et al. (1986).

2. QUANTUM-MECHANICAL METHOD

Explicit quantum-mechanical scattering calculations of rovibrational transition cross sections for a heavy diatomic molecule such as CO is a computationally challenging problem, especially when transitions among highly excited rovibrational levels are involved. To reduce the computational effort, we use the infinite-order sudden (IOS) approximation for obtaining the vibrational transition cross sections, which is a good approximation at high collision energies. For the rotational transitions, we use explicit coupled-channel scattering calculations (Arthurs & Dalgarno 1960).

The rate coefficient for a given rovibrational transition is obtained by averaging the appropriate cross section over a Boltzmann distribution of velocities of the incoming atom at a specified temperature T,

$$k_{v,j \to v',j'}(T) = (8/\pi\mu\beta)^{1/2}\beta^2$$
$$\times \int_0^\infty E_k \sigma_{v,j \to v',j'}(E_k) \exp(-\beta E_k)\, dE_k , \quad (1)$$

where $\sigma_{v,j \to v',j'}$ is the rovibrational transition cross section with vj and $v'j'$ being respectively the initial and final vibrational/rotational quantum numbers, μ is the reduced mass of the system, E_k is the kinetic energy, and $\beta = (k_B T)^{-1}$,

where k_B is the Boltzmann constant. The rate coefficient for the reverse transition can be obtained by detailed balance:

$$k_{v'j'\to vj}(T) = \frac{(2j+1)}{(2j'+1)}\exp[\beta(\epsilon_{v'j'} - \epsilon_{vj})]k_{v,j\to v',j'}(T). \quad (2)$$

The MOLSCAT program developed by Hutson & Green (1994) was used to perform the scattering calculations for both vibrational and rotational transitions.

3. RESULTS

First we describe the rotational transition calculations. The rotational transition cross sections are strongly influenced by the anisotropy of the interaction potential with respect to the angle of approach of the H atom to the center of mass of the CO molecule. In the scattering calculations, the angular dependence of the interaction potential is represented as an expansion in Legendre polynomials. Due to the strong anisotropy of the H-CO interaction potential, we have retained terms of all orders up to 20 in the Legendre expansion.

Fully closed-coupled scattering calculations were performed for total energy values ranging from $E = 0.01$ to 6000 cm^{-1}. The basis set employed in these calculations includes rotational levels $j = 0$–35 within the $v = 0$ manifold, with energies presented in Table 1. The energy of the highest rotational level considered is 2396 cm^{-1}, and our calculation excludes channels that are open at total energy values above this energy. This is not a major source of error in the calculation for which the highest temperature is 3000 K, and rotational levels above $j = 35$ are not significantly populated. Sufficient total angular momentum partial waves J were included to ensure the convergence of the individual cross sections. The highest value of J retained is 90.

It has been shown by Green et al. (1996) that the rotational excitation cross sections computed using the potential-energy surface of Keller et al. (1996; referred to as WKS) differ significantly from those obtained using the surface of Bowman et al. (1986; referred to as BBH). The difference was most notable for the $j = 0 \to 1$ transition, in which the newer WKS potential yields cross sections that are a factor of 6 larger than those obtained using the BBH surface (Green et al. 1996). The comparisons were made at a kinetic energy of 3000 cm^{-1}, and the difference was attributed to the long-range part of the H-CO interaction potential, which was better described by the WKS potential. We find that the discrepancies are even larger at lower kinetic energies, at which the long-range interaction becomes still more important. This is illustrated in Figure 1, in which we compare the cross sections for pure rotational excitations out of the $v = 0$, $j = 0$ level obtained from the WKS potential and the BBH surface as functions of the final rotational quantum number. Figure 1a compares the cross sections for different rotational transitions at an incident kinetic energy of 400 cm^{-1} and Figure 1b at an energy of 800 cm^{-1}. The data for the BBH potential are taken from Green et al. (1995). The $j = 0 \to 1$ excitation cross section obtained using the WKS potential is about a factor of 30 larger than that obtained using the BBH potential at an energy of 400 cm^{-1} and about a factor of 10 larger at an energy of 800 cm^{-1}. The greater discrepancy at the smaller incident energy is consistent with the increased contribution of the long-range interaction at low incident velocities. Although the BBH

TABLE 1
CO ROTATIONAL ENERGIES

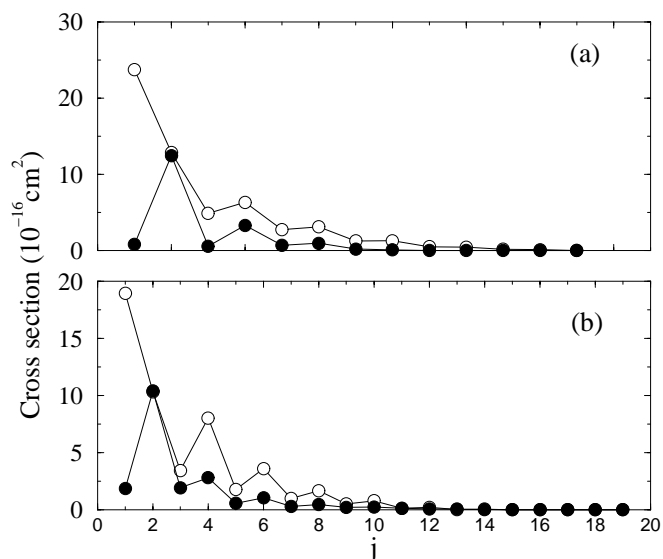| j	ϵ_j (cm^{-1})
0	0.0
1	3.8
2	11.5
3	22.9
4	38.2
5	57.3
6	80.2
7	106.9
8	137.4
9	171.8
10	209.9
11	251.9
12	297.7
13	347.3
14	400.7
15	457.9
16	518.9
17	583.7
18	652.2
19	724.6
20	800.8
21	880.8
22	964.5
23	1052.0
24	1143.4
25	1238.4
26	1337.3
27	1439.9
28	1546.3
29	1656.5
30	1770.4
31	1888.0
32	2009.4
33	2134.6
34	2263.5
35	2396.0

FIG. 1.—Comparison of rotational excitation cross sections from the $j = 0$ level of CO by collisions with H from the present study (*open circles*) and those of Green et al. (1995) using the BBH potential-energy surface (*filled circles*). (*a*) At an incident kinetic energy of 400 cm^{-1}; (*b*) at an incident kinetic energy of 800 cm^{-1}.

TABLE 2
Pure Rotational Quenching Rate Coefficients $k_{j \to j'}(T)$ for CO in Collision with H as Functions
of Temperature

T (K)	$1 \to 0$	$2 \to 1$	$2 \to 0$	$3 \to 2$	$3 \to 1$	$3 \to 0$	$4 \to 3$
5.........	0.178E−09	0.341E−09	0.974E−10	0.358E−09	0.186E−09	0.398E−10	0.294E−09
10.......	0.193E−09	0.342E−09	0.931E−10	0.377E−09	0.173E−09	0.333E−10	0.328E−09
20.......	0.202E−09	0.323E−09	0.825E−10	0.370E−09	0.148E−09	0.242E−10	0.347E−09
30.......	0.209E−09	0.314E−09	0.769E−10	0.362E−09	0.136E−09	0.197E−10	0.351E−09
40.......	0.215E−09	0.311E−09	0.741E−10	0.357E−09	0.130E−09	0.174E−10	0.353E−09
50.......	0.220E−09	0.311E−09	0.726E−10	0.355E−09	0.126E−09	0.160E−10	0.355E−09
60.......	0.225E−09	0.312E−09	0.718E−10	0.354E−09	0.124E−09	0.153E−10	0.356E−09
70.......	0.228E−09	0.313E−09	0.715E−10	0.353E−09	0.123E−09	0.148E−10	0.357E−09
80.......	0.232E−09	0.314E−09	0.713E−10	0.353E−09	0.122E−09	0.146E−10	0.358E−09
90.......	0.234E−09	0.314E−09	0.711E−10	0.352E−09	0.122E−09	0.145E−10	0.357E−09
100......	0.237E−09	0.315E−09	0.710E−10	0.350E−09	0.121E−09	0.144E−10	0.356E−09

T (K)	$4 \to 2$	$4 \to 1$	$4 \to 0$	$5 \to 4$	$5 \to 3$	$5 \to 2$	$5 \to 1$
5.........	0.168E−09	0.958E−10	0.392E−10	0.255E−09	0.126E−09	0.835E−10	0.663E−10
10.......	0.166E−09	0.846E−10	0.348E−10	0.286E−09	0.131E−09	0.796E−10	0.623E−10
20.......	0.152E−09	0.656E−10	0.283E−10	0.315E−09	0.130E−09	0.688E−10	0.543E−10
30.......	0.144E−09	0.548E−10	0.249E−10	0.328E−09	0.129E−09	0.610E−10	0.493E−10
40.......	0.140E−09	0.482E−10	0.230E−10	0.335E−09	0.129E−09	0.558E−10	0.462E−10
50.......	0.138E−09	0.441E−10	0.218E−10	0.341E−09	0.130E−09	0.524E−10	0.441E−10
60.......	0.137E−09	0.414E−10	0.210E−10	0.344E−09	0.131E−09	0.499E−10	0.426E−10
70.......	0.137E−09	0.395E−10	0.204E−10	0.347E−09	0.132E−09	0.482E−10	0.415E−10
80.......	0.136E−09	0.381E−10	0.200E−10	0.348E−09	0.133E−09	0.469E−10	0.406E−10
90.......	0.136E−09	0.371E−10	0.197E−10	0.349E−09	0.134E−09	0.458E−10	0.398E−10
100......	0.136E−09	0.363E−10	0.194E−10	0.348E−09	0.134E−09	0.448E−10	0.391E−10

T (K)	$5 \to 0$	$6 \to 5$	$6 \to 4$	$6 \to 3$	$6 \to 2$	$6 \to 1$	$6 \to 0$
5.........	0.230E−10	0.229E−09	0.983E−10	0.676E−10	0.567E−10	0.328E−10	0.126E−10
10.......	0.211E−10	0.252E−09	0.104E−09	0.676E−10	0.565E−10	0.316E−10	0.119E−10
20.......	0.175E−10	0.283E−09	0.109E−09	0.638E−10	0.539E−10	0.285E−10	0.107E−10
30.......	0.150E−10	0.301E−09	0.113E−09	0.597E−10	0.516E−10	0.260E−10	0.991E−11
40.......	0.134E−10	0.312E−09	0.116E−09	0.566E−10	0.499E−10	0.242E−10	0.936E−11
50.......	0.122E−10	0.320E−09	0.119E−09	0.543E−10	0.487E−10	0.228E−10	0.896E−11
60.......	0.114E−10	0.326E−09	0.121E−09	0.525E−10	0.479E−10	0.217E−10	0.865E−11
70.......	0.107E−10	0.330E−09	0.124E−09	0.511E−10	0.472E−10	0.208E−10	0.840E−11
80.......	0.102E−10	0.332E−09	0.125E−09	0.499E−10	0.465E−10	0.201E−10	0.818E−11
90.......	0.983E−11	0.333E−09	0.127E−09	0.489E−10	0.459E−10	0.194E−10	0.798E−11
100......	0.948E−11	0.332E−09	0.127E−09	0.479E−10	0.452E−10	0.189E−10	0.780E−11

T (K)	$7 \to 6$	$7 \to 5$	$7 \to 4$	$7 \to 3$	$7 \to 2$	$7 \to 1$	$7 \to 0$
5.........	0.208E−09	0.808E−10	0.565E−10	0.434E−10	0.277E−10	0.187E−10	0.562E−11
10.......	0.224E−09	0.855E−10	0.577E−10	0.451E−10	0.278E−10	0.182E−10	0.536E−11
20.......	0.253E−09	0.931E−10	0.578E−10	0.464E−10	0.274E−10	0.177E−10	0.503E−11
30.......	0.273E−09	0.986E−10	0.566E−10	0.467E−10	0.265E−10	0.172E−10	0.476E−11
40.......	0.287E−09	0.103E−09	0.553E−10	0.467E−10	0.256E−10	0.168E−10	0.454E−11
50.......	0.297E−09	0.108E−09	0.541E−10	0.467E−10	0.248E−10	0.165E−10	0.437E−11
60.......	0.304E−09	0.111E−09	0.532E−10	0.466E−10	0.242E−10	0.162E−10	0.422E−11
70.......	0.309E−09	0.115E−09	0.523E−10	0.465E−10	0.235E−10	0.159E−10	0.409E−11
80.......	0.312E−09	0.117E−09	0.514E−10	0.463E−10	0.229E−10	0.156E−10	0.397E−11
90.......	0.313E−09	0.118E−09	0.505E−10	0.459E−10	0.224E−10	0.154E−10	0.386E−11
100......	0.312E−09	0.119E−09	0.496E−10	0.454E−10	0.218E−10	0.151E−10	0.375E−11

Note.—Coefficients are in units of $cm^3\,s^{-1}$.

potential was constructed to reproduce the main spectroscopic features of the HCO radical, no special attention was given to the long-range part of the H-CO van der Waals interaction in constructing the potential. Our results for the $j = 0 \to 1$ excitation are in somewhat better agreement with those obtained by Chu & Dalgarno (1975) using a model potential that takes into account the long-range interaction. Using a coupled-states approximation for the scattering calculations, Chu & Dalgarno obtained a value of 8.85 $Å^2$

for the $j = 0 \to 1$ excitation cross section at an energy of 400 cm^{-1}, which is a factor of 3 smaller than the present results. Our convergence calculations, as well as those of Chu & Dalgarno (1975) and Green et al. (1995), show that the coupled-states approximation gives cross sections within 10% of the exact coupled-channel results.

Green & Thaddeus (1976) have reported rate coefficients for pure rotational deexcitation transitions in the temperature range of 5–100 K for the lowest eight rotational levels

TABLE 3
PURE ROTATIONAL QUENCHING RATE COEFFICIENTS $k_{j \to j'}(T)$
FOR CO IN COLLISION WITH H AS FUNCTIONS OF TEMPERATURE

This table is available only on-line as a machine-readable table.

TABLE 4
CO VIBRATIONAL
ENERGIES

v	ϵ_v (cm^{-1})
0......................	1082
1......................	3227
2......................	5345
3......................	7438
4......................	9505
5......................	11545
6......................	13560
7......................	15548
8......................	17511
9......................	19447

of the CO molecule. In Table 2 we present our results for these rate coefficients in the same temperature range. The corresponding excitation rate coefficients can be derived by detailed balance using equation (2). Our results differ significantly from the results of Green & Thaddeus (1976), which have been widely employed in modeling CO emission lines in interstellar molecular clouds. For example, for the $j = 1 \to 0$ transition at 100 K, we obtain a value of 2.4×10^{-10} cm^3 s^{-1} for the rate coefficient, compared to the value of 7×10^{-12} cm^3 s^{-1} obtained by Green & Thaddeus. At a temperature of 10 K, our value is 1.9×10^{-10} cm^3 s^{-1}, compared to 6.7×10^{-12} cm^3 s^{-1} obtained by Green & Thaddeus for the same transition. Thus, our values are about 30 times larger than those of Green & Thaddeus (1976) for the $j = 1 \to 0$ transition at low temperatures. The discrepancies are a reflection of the differences in the interaction potentials employed. The potential surface used here, based on more realistic and elaborate ab initio calculations and tested against spectroscopic data (Tobiason et al. 1995; Keller et al. 1996; Green et al. 1996), should give a better description of the H-CO interaction.

In Table 3 we present rate coefficients for pure rotational deexcitation among the first 17 rotational levels in the temperature range 100–3000 K. The rate coefficient decreases with increasing $\Delta j = j - j'$, as expected. Rate coefficients for $|\Delta j| = 1$ transitions originating from excited rotational levels are comparable in magnitude to the $j = 1 \to 0$ transition because the same anisotropic part of the interaction poten-

tial is mainly responsible for driving these transitions. However, due to the availability of additional excitation or deexcitation channels for excited rotational levels, the transition intensities are slightly lower compared to the $j = 1 \to 0$ transition.

The vibrational transition rate coefficients are more difficult to calculate owing to the large number of vibrational levels and the numerous rotational levels in each vibrational manifold. An exact coupled-channel calculation or coupled-states calculation is prohibitively expensive in calculating vibrational transition rate coefficients. Hence, we have resorted to the IOS approximation, in which the couplings between rotational levels are omitted and a set of coupled equations in a basis of vibrational levels of the molecule is solved for a fixed angle of approach of the H atom to the center of mass of the CO molecule (Tsien & Park 1970). Results are subsequently averaged over all possible

TABLE 5
VIBRATIONAL QUENCHING RATE COEFFICIENTS $k_{v \to v'}(T)$ FOR CO IN COLLISION WITH H AS FUNCTIONS OF TEMPERATURE

T (K)	$1 \to 0$	$2 \to 1$	$2 \to 0$	$3 \to 2$	$3 \to 1$	$3 \to 0$	$4 \to 3$
100......	0.220E−14	0.269E−14	0.470E−15	0.347E−14	0.139E−14	0.302E−15	0.251E−14
200......	0.666E−13	0.667E−13	0.160E−13	0.707E−13	0.387E−13	0.871E−14	0.661E−13
300......	0.379E−12	0.392E−12	0.105E−12	0.404E−12	0.233E−12	0.515E−13	0.388E−12
500......	0.213E−11	0.238E−11	0.689E−12	0.233E−11	0.139E−11	0.315E−12	0.217E−11
700......	0.516E−11	0.596E−11	0.181E−11	0.565E−11	0.347E−11	0.824E−12	0.500E−11
1000....	0.110E−10	0.129E−10	0.420E−11	0.120E−10	0.755E−11	0.194E−11	0.108E−10
1500....	0.223E−10	0.257E−10	0.920E−11	0.236E−10	0.151E−10	0.439E−11	0.209E−10
2000....	0.340E−10	0.379E−10	0.147E−10	0.344E−10	0.220E−10	0.709E−11	0.293E−10
2500....	0.455E−10	0.487E−10	0.199E−10	0.433E−10	0.276E−10	0.953E−11	0.352E−10
3000....	0.561E−10	0.575E−10	0.246E−10	0.498E−10	0.317E−10	0.115E−10	0.387E−10

T (K)	$4 \to 2$	$4 \to 1$	$4 \to 0$
100......	0.150E−14	0.717E−15	0.109E−15
200......	0.510E−13	0.240E−13	0.356E−14
300......	0.306E−12	0.144E−12	0.223E−13
500......	0.174E−11	0.863E−12	0.145E−12
700......	0.417E−11	0.216E−11	0.392E−12
1000....	0.868E−11	0.472E−11	0.955E−12
1500....	0.163E−10	0.936E−11	0.217E−11
2000....	0.223E−10	0.132E−10	0.335E−11
2500....	0.262E−10	0.158E−10	0.424E−11
3000....	0.284E−10	0.173E−10	0.484E−11

NOTE.—Coefficients are in units of cm^3 s^{-1}.

angles of approach: we used 100 Gauss-Legendre quadrature points as the angle variable in the quadrature scheme employed to perform the averaging.

We used the Morse potential for CO in computing the matrix elements of the interaction potential between the vibrational wave functions. We included the first 10 vibrational states in our basis set with the energy levels given in Table 4. These 10 levels are sufficient to secure convergence. Cross sections were computed for 65 energies in the range 2200–16,000 cm^{-1}. Vibrational excitations of CO by H atoms were studied by Green et al. (1995) using the BBH potential and by Green et al. (1996) using the WKS potential. The latter study was restricted to two values of the kinetic energy: 3000 and 18,550 cm^{-1}. The vibrational excitation cross sections are less sensitive to the details of the potential, and the two potentials yielded comparable results. This is not surprising, because vibrational transitions involve much larger energies than rotational transitions, and the main contribution comes from head-on collisions. Our result for the $v = 0 \rightarrow 1$ excitation cross section at a kinetic energy of 3000 cm^{-1} is in good agreement with that reported by Green et al. (1996).

In Table 5 we present rate coefficients for vibrational quenching of the first five vibrational levels for temperatures ranging from 100 to 3000 K. The $v = 1 \rightarrow 0$ values are in good agreement with the experimental results of Glass & Kironde (1982) as estimated by Ayres & Wiedemann (1989). The corresponding excitation rate coefficients can be derived by detailed balance.

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