# Rate coefficients for the rotational excitation of CO by ortho- and para-H2

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# Rate coefficients for the rotational excitation of CO by *ortho*- and *para*-$H_2$

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**Summary.** Rate coefficients for the rotational excitation of $^{12}C^{16}O$ by *ortho*- and *para*-$H_2$ are given for the low-temperature regime of interstellar molecular clouds. The rate coefficients derive from quantum mechanical coupled channels calculations of the relevant cross-sections and are intended for the analysis of the intensities of CO microwave and submillimetre lines.

## 1 Introduction

Rate coefficients for rotational excitation by $H_2$ are required to interpret the microwave and submillimetre spectra of interstellar molecules. Of particular importance, in view of its high abundance and ease of observation, is the CO molecule. Whilst a number of studies of the rotational excitation of CO by He have been made (Green & Thaddeus 1976; Green & Chapman 1978; Thomas, Kraemer & Diercksen 1980; McKee *et al.* 1982), cross-sections for the excitation of CO by $H_2$ have not been explicitly calculated. Cross-sections and rate coefficients for excitation by *para*-$H_2$ have been obtained by scaling the CO–He interaction potential (Green & Thaddeus 1976). Even simpler scaling procedures, which account only for the greater velocity of the $H_2$ molecule at a given collision energy, are often used to derive rate coefficients for *para*-$H_2$ from the results of calculations for excitation by He (*cf.* McKee *et al.* 1982). Such procedures are of uncertain accuracy and do not yield results for *ortho*-$H_2$ which may be the more abundant modification.

In the present paper, we tabulate the results of calculations of rate coefficients for the rotational excitation of $^{12}C^{16}O$ by both *para*- and *ortho*-$H_2$. They are based on an *ab initio* calculation of the CO–$H_2$ interaction potential and quantum mechanical coupled channels calculations of the rotational excitation cross-sections. Comparisons are made with the results of Green & Thaddeus (1976), at low temperatures ($T \leqslant 100$ K). Limited comparison is also possible with calculations at higher temperatures ($T > 100$ K) by McKee *et al.* (1982).

## 2 Details of calculations

The quantum mechanical coupled channels (CC) technique is well documented, and the particular formalism relevant to the present calculations has been given by Launay (1977). No

dynamical approximations were made in these calculations, and the accuracy of the final results is determined by (i) the precision of the intermolecular potential and (ii) the sizes of the rotational basis sets.

## 2.1 INTERMOLECULAR POTENTIAL

The CO–$H_2$ interaction potential employed is that described by Prissette, Kochanski & Flower (1978) and Flower *et al.* (1979). This potential was computed by *ab initio* methods using double zeta basis sets and polarization functions. The limited size of the basis sets used in the calculation gave rise to superposition errors whose consequences for the rotational excitation have been established in comparison with double resonance (Brechignac *et al.* 1980), line broadening (Picard-Bersellini, Charneau & Brechignac 1983), and differential scattering (Andres *et al.* 1982; Schinke *et al.* 1984) data. These comparisons show the depth of the well in the isotropic part of the potential to be overestimated but suggest that the anisotropic part of the interaction is predicted to reasonable accuracy. Consequently the data presented below are principally recommended for use when interpreting the *relative* intensities of rotationally inelastic transitions within the $^{12}C^{16}O$ molecule. The data may also be used in studies of isotopic spectra ($^{13}C^{16}O$, $^{12}C^{18}O$), as the corresponding displacements of the centre of mass are not large.

## 2.2 ROTATIONAL BASIS SETS

### 2.2.1 $H_2$

The $H_2$ molecule exists in either the *para-* (even $j$) or *ortho-* (odd $j$) modifications. The relative abundance of the two species is dependent on the cloud chemistry (Flower & Watt 1984) and is unknown in dense clouds. At the low temperatures which are believed to characterize dense molecular clouds (except in the wake of a shock), the two modifications may be expected to be in their ground states. Furthermore, the energy gaps between $j=0$ and $j=2$, in *para*-$H_2$, and $j=1$ and $j=3$, in *ortho*-$H_2$, are sufficiently large (510 and 845 K respectively) compared with the thermal kinetic energy ($T<100$ K) that the effects of closed channels ($j>1$) on cross-sections for rotational excitation of CO may be expected to be small. Accordingly, we have adopted minimal rotational bases for $H_2$, namely $j=0$ for *para*-$H_2$ and $j=1$ for *ortho*-$H_2$. We note that, subject to these approximations, long-range interactions with the multipole moments of the $H_2$ molecule are present in the case of *ortho*-$H_2$ but are absent in the case of *para*-$H_2$.

### 2.2.2 $^{12}C^{16}O$

As CO is a heavy molecule, its rotational constant is small ($B_0=1.92265\ cm^{-1}$; Herzberg 1950) and many rotational levels are energetically accessible even at modest kinetic temperatures. For this reason, extended rotational basis sets are necessary for the CO molecule, including energetically closed rotational levels. Denoting by B$n$ a rotational basis set comprising $J=0, 1, 2, \ldots, n$, the following basis sets have been used as functions of the total (internal rotational plus relative kinetic) barycentric energy, $E$: for collisions with *para*-$H_2$ ($j=0$), B7 for $0<E<80$ K, B8 for $80<E<200$ K, B11 for $200<E<500$ K, and B12 for $E>500$ K; for collisions with *ortho*-$H_2$ ($j=1$), B5 for $0<E<100$ K, B6 for $E>100$ K.

For a given CO rotational basis set, the computational time is much greater for collisions with *ortho-* than with *para*-$H_2$, owing to the coupling with the rotational angular momentum of the $H_2$ molecule. For this reason we have adopted smaller rotational bases for calculations involving the excitation of CO by *ortho*-$H_2$. Accordingly, rate coefficients for excitation by *ortho*-$H_2$ are given for $T<100$ K, whereas results for *para*-$H_2$ extend to $T=250$ K.

**Table 1.** Rate coefficients, $q(J \rightarrow J')$, for rotational de-excitation of $^{12}C^{16}O$ by *para*-$H_2$, in units of $cm^3 s^{-1}$. Numbers in parentheses are powers of 10.

| J | J' | T(K) | | | | | |
|---|---|---|---|---|---|---|---|
| | | 10 | 20 | 40 | 60 | 100 | 250 |
| 1 | 0 | 2.3(-11) | 2.4(-11) | 3.3(-11) | 4.1(-11) | 5.0(-11) | 5.8(-11) |
| 2 | 0 | 3.5(-11) | 3.8(-11) | 4.2(-11) | 4.5(-11) | 4.7(-11) | 5.1(-11) |
| 3 | 0 | 2.8(-12) | 3.8(-12) | 4.9(-12) | 5.8(-12) | 7.2(-12) | 1.0(-11) |
| 4 | 0 | 3.8(-12) | 4.7(-12) | 5.7(-12) | 6.2(-12) | 6.8(-12) | 8.1(-12) |
| 5 | 0 | 6.2(-13) | 7.4(-13) | 1.0(-12) | 1.3(-12) | 2.0(-12) | 4.2(-12) |
| 6 | 0 | 5.9(-13) | 7.0(-13) | 9.1(-13) | 1.1(-12) | 1.4(-12) | 2.1(-12) |
| 7 | 0 | 1.8(-13) | 2.1(-13) | 2.8(-13) | 3.6(-13) | 5.8(-13) | 1.6(-12) |
| 8 | 0 | 1.3(-13) | 1.7(-13) | 2.2(-13) | 2.8(-13) | 4.0(-13) | 8.6(-13) |
| 9 | 0 | 4.1(-14) | 5.7(-14) | 7.8(-14) | 1.0(-13) | 1.8(-13) | 6.0(-13) |
| 10 | 0 | 2.4(-14) | 3.5(-14) | 5.0(-14) | 6.7(-14) | 1.1(-13) | 3.6(-13) |
| 11 | 0 | 9.3(-15) | 1.4(-14) | 2.2(-14) | 3.2(-14) | 6.0(-14) | 2.2(-13) |
| 2 | 1 | 2.8(-11) | 3.5(-11) | 4.9(-11) | 6.0(-11) | 7.3(-11) | 8.7(-11) |
| 3 | 1 | 6.2(-11) | 6.6(-11) | 7.1(-11) | 7.3(-11) | 7.5(-11) | 8.1(-11) |
| 4 | 1 | 5.0(-12) | 8.0(-12) | 1.1(-11) | 1.3(-11) | 1.5(-11) | 2.1(-11) |
| 5 | 1 | 7.2(-12) | 7.9(-12) | 9.4(-12) | 1.1(-11) | 1.2(-11) | 1.5(-11) |
| 6 | 1 | 1.4(-12) | 1.8(-12) | 2.4(-12) | 3.0(-12) | 4.2(-12) | 8.6(-12) |
| 7 | 1 | 1.2(-12) | 1.4(-12) | 1.8(-12) | 2.1(-12) | 2.7(-12) | 4.4(-12) |
| 8 | 1 | 3.5(-13) | 4.6(-13) | 6.1(-13) | 7.8(-13) | 1.2(-12) | 3.3(-12) |
| 9 | 1 | 2.7(-13) | 3.5(-13) | 4.6(-13) | 5.7(-13) | 8.1(-13) | 1.8(-12) |
| 10 | 1 | 7.7(-14) | 1.1(-13) | 1.6(-13) | 2.1(-13) | 3.7(-13) | 1.3(-12) |
| 11 | 1 | 5.6(-14) | 8.1(-14) | 1.2(-13) | 1.6(-13) | 2.6(-13) | 7.5(-13) |
| 3 | 2 | 2.5(-11) | 3.9(-11) | 5.9(-11) | 7.0(-11) | 8.3(-11) | 9.8(-11) |
| 4 | 2 | 7.4(-11) | 8.1(-11) | 8.7(-11) | 8.9(-11) | 8.9(-11) | 9.3(-11) |
| 5 | 2 | 6.3(-12) | 7.7(-12) | 1.1(-11) | 1.3(-11) | 1.7(-11) | 2.6(-11) |
| 6 | 2 | 1.1(-11) | 1.1(-11) | 1.3(-11) | 1.4(-11) | 1.5(-11) | 1.8(-11) |
| 7 | 2 | 2.3(-12) | 2.6(-12) | 3.3(-12) | 3.9(-12) | 5.4(-12) | 1.1(-11) |
| 8 | 2 | 1.6(-12) | 2.0(-12) | 2.5(-12) | 2.9(-12) | 3.6(-12) | 5.7(-12) |
| 9 | 2 | 5.1(-13) | 6.8(-13) | 9.0(-13) | 1.1(-12) | 1.7(-12) | 4.3(-12) |
| 10 | 2 | 3.0(-13) | 4.2(-13) | 5.8(-13) | 7.3(-13) | 1.0(-12) | 2.3(-12) |
| 11 | 2 | 1.2(-13) | 1.8(-13) | 2.8(-13) | 3.8(-13) | 6.3(-13) | 1.7(-12) |
| 4 | 3 | 3.2(-11) | 4.7(-11) | 6.5(-11) | 7.6(-11) | 8.7(-11) | 1.0(-10) |
| 5 | 3 | 8.9(-11) | 9.2(-11) | 9.6(-11) | 9.7(-11) | 9.7(-11) | 1.0(-10) |
| 6 | 3 | 9.3(-12) | 1.1(-11) | 1.4(-11) | 1.7(-11) | 2.0(-11) | 2.9(-11) |
| 7 | 3 | 1.3(-11) | 1.4(-11) | 1.5(-11) | 1.6(-11) | 1.7(-11) | 2.0(-11) |
| 8 | 3 | 2.6(-12) | 3.4(-12) | 4.3(-12) | 5.1(-12) | 6.8(-12) | 1.3(-11) |
| 9 | 3 | 2.0(-12) | 2.6(-12) | 3.2(-12) | 3.6(-12) | 4.3(-12) | 6.3(-12) |
| 10 | 3 | 6.3(-13) | 8.9(-13) | 1.2(-12) | 1.5(-12) | 2.3(-12) | 5.2(-12) |
| 11 | 3 | 4.2(-13) | 6.1(-13) | 8.7(-13) | 1.1(-12) | 1.5(-12) | 2.8(-12) |
| 5 | 4 | 4.0(-11) | 5.0(-11) | 6.5(-11) | 7.6(-11) | 8.8(-11) | 1.0(-10) |
| 6 | 4 | 1.0(-10) | 1.0(-10) | 1.1(-10) | 1.1(-10) | 1.0(-10) | 1.1(-10) |
| 7 | 4 | 1.7(-11) | 1.7(-11) | 1.9(-11) | 2.0(-11) | 2.3(-11) | 3.1(-11) |
| 8 | 4 | 1.3(-11) | 1.6(-11) | 1.8(-11) | 1.9(-11) | 2.0(-11) | 2.2(-11) |
| 9 | 4 | 3.4(-12) | 4.5(-12) | 5.6(-12) | 6.4(-12) | 8.0(-12) | 1.4(-11) |
| 10 | 4 | 1.9(-12) | 2.6(-12) | 3.4(-12) | 3.9(-12) | 4.8(-12) | 6.9(-12) |
| 11 | 4 | 8.7(-13) | 1.3(-12) | 1.9(-12) | 2.4(-12) | 3.4(-12) | 6.4(-12) |
| 6 | 5 | 5.1(-11) | 6.0(-11) | 7.6(-11) | 8.5(-11) | 9.4(-11) | 1.0(-10) |
| 7 | 5 | 1.0(-10) | 1.1(-10) | 1.1(-10) | 1.1(-10) | 1.1(-10) | 1.1(-10) |
| 8 | 5 | 1.3(-11) | 1.7(-11) | 2.1(-11) | 2.3(-11) | 2.6(-11) | 3.4(-11) |
| 9 | 5 | 1.3(-11) | 1.7(-11) | 2.0(-11) | 2.0(-11) | 2.1(-11) | 2.3(-11) |
| 10 | 5 | 3.8(-12) | 5.4(-12) | 7.1(-12) | 8.3(-12) | 1.0(-11) | 1.6(-11) |
| 11 | 5 | 2.2(-12) | 3.2(-12) | 4.4(-12) | 5.2(-12) | 6.4(-12) | 8.2(-12) |
| 7 | 6 | 8.5(-11) | 8.4(-11) | 8.8(-11) | 9.2(-11) | 9.8(-11) | 1.1(-10) |
| 8 | 6 | 9.0(-11) | 1.1(-10) | 1.2(-10) | 1.2(-10) | 1.2(-10) | 1.1(-10) |
| 9 | 6 | 1.5(-11) | 2.0(-11) | 2.3(-11) | 2.5(-11) | 2.7(-11) | 3.5(-11) |
| 10 | 6 | 1.1(-11) | 1.5(-11) | 1.8(-11) | 2.0(-11) | 2.1(-11) | 2.4(-11) |
| 11 | 6 | 4.8(-12) | 7.0(-12) | 9.9(-12) | 1.2(-11) | 1.5(-11) | 2.1(-11) |

**Table 1** – *continued*

| J | J' | T(K) | | | | | |
|---|---|---|---|---|---|---|---|
| | | 10 | 20 | 40 | 60 | 100 | 250 |
| 8 | 7 | 4.5(-11) | 6.8(-11) | 8.5(-11) | 9.2(-11) | 9.7(-11) | 1.0(-10) |
| 9 | 7 | 7.8(-11) | 1.0(-10) | 1.1(-10) | 1.2(-10) | 1.1(-10) | 1.1(-10) |
| 10 | 7 | 1.5(-11) | 2.2(-11) | 2.8(-11) | 3.1(-11) | 3.6(-11) | 4.2(-11) |
| 11 | 7 | 1.1(-11) | 1.6(-11) | 2.0(-11) | 2.3(-11) | 2.5(-11) | 2.8(-11) |
| 9 | 8 | 4.0(-11) | 5.6(-11) | 7.2(-11) | 8.0(-11) | 8.8(-11) | 1.0(-10) |
| 10 | 8 | 5.5(-11) | 8.0(-11) | 9.8(-11) | 1.0(-10) | 1.1(-10) | 1.1(-10) |
| 11 | 8 | 1.7(-11) | 2.5(-11) | 3.5(-11) | 4.0(-11) | 4.7(-11) | 5.4(-11) |
| 10 | 9 | 3.2(-11) | 5.0(-11) | 7.0(-11) | 8.3(-11) | 9.7(-11) | 1.1(-10) |
| 11 | 9 | 5.6(-11) | 8.4(-11) | 1.1(-10) | 1.2(-10) | 1.2(-10) | 1.3(-10) |
| 11 | 10 | 2.8(-11) | 4.5(-11) | 6.6(-11) | 8.0(-11) | 9.7(-11) | 1.2(-10) |

In Table 1, rate coefficients for the rotational *de*-excitation of $^{12}C^{16}O$ by *para*-$H_2$ are given as functions of the kinetic temperature, $T$. Results for transitions involving large values of $J$ are less reliable than for small $J$ owing to (i) the progressive insufficiency of the rotational basis sets, and (ii) the smaller number of collision energies at which the corresponding cross-sections were calculated. Results for excitation by *ortho*-$H_2$ are given in Table 2. Owing to the long-range multipolar interaction between CO and *ortho*-$H_2$, rate coefficients for *ortho*-$H_2$ tend to be larger than for *para*-$H_2$, particularly at low temperatures.

Rate coefficients for rotational excitation may be derived from the principle of detailed

**Table 2.** Rate coefficients, $q(J \rightarrow J')$, for rotational de-excitation of $^{12}C^{16}O$ by *ortho*-$H_2$, in units of $cm^3 s^{-1}$. Numbers in parentheses are powers of 10.

| J | J' | T(K) | | | | | |
|---|---|---|---|---|---|---|---|
| | | 10 | 20 | 40 | 60 | 80 | 100 |
| 1 | 0 | 5.5(-11) | 4.5(-11) | 4.5(-11) | 4.9(-11) | 5.3(-11) | 5.7(-11) |
| 2 | 0 | 7.7(-11) | 7.4(-11) | 6.9(-11) | 6.6(-11) | 6.5(-11) | 6.4(-11) |
| 3 | 0 | 5.3(-12) | 5.9(-12) | 6.6(-12) | 7.0(-12) | 7.4(-12) | 7.7(-12) |
| 4 | 0 | 1.1(-11) | 1.1(-11) | 1.1(-11) | 1.1(-11) | 1.1(-11) | 1.1(-11) |
| 5 | 0 | 1.5(-12) | 1.8(-12) | 2.2(-12) | 2.5(-12) | 2.7(-12) | 2.9(-12) |
| 6 | 0 | 1.5(-12) | 1.7(-12) | 2.0(-12) | 2.2(-12) | 2.4(-12) | 2.6(-12) |
| 2 | 1 | 6.6(-11) | 6.4(-11) | 6.7(-11) | 7.2(-11) | 7.7(-11) | 8.2(-11) |
| 3 | 1 | 1.1(-10) | 1.1(-10) | 1.1(-10) | 1.1(-10) | 1.1(-10) | 1.0(-10) |
| 4 | 1 | 9.9(-12) | 1.3(-11) | 1.5(-11) | 1.5(-11) | 1.6(-11) | 1.6(-11) |
| 5 | 1 | 1.8(-11) | 1.9(-11) | 1.9(-11) | 2.0(-11) | 2.0(-11) | 2.0(-11) |
| 6 | 1 | 2.8(-12) | 3.5(-12) | 4.6(-12) | 5.5(-12) | 6.2(-12) | 6.8(-12) |
| 3 | 2 | 5.1(-11) | 6.1(-11) | 7.1(-11) | 7.8(-11) | 8.4(-11) | 8.9(-11) |
| 4 | 2 | 1.2(-10) | 1.2(-10) | 1.2(-10) | 1.2(-10) | 1.2(-10) | 1.2(-10) |
| 5 | 2 | 8.7(-12) | 1.2(-11) | 1.7(-11) | 2.0(-11) | 2.2(-11) | 2.4(-11) |
| 6 | 2 | 2.1(-11) | 2.2(-11) | 2.4(-11) | 2.5(-11) | 2.6(-11) | 2.7(-11) |
| 4 | 3 | 4.6(-11) | 5.7(-11) | 7.2(-11) | 8.1(-11) | 8.8(-11) | 9.4(-11) |
| 5 | 3 | 1.3(-10) | 1.3(-10) | 1.3(-10) | 1.3(-10) | 1.3(-10) | 1.3(-10) |
| 6 | 3 | 1.1(-11) | 1.4(-11) | 2.1(-11) | 2.5(-10) | 2.9(-11) | 3.2(-11) |
| 5 | 4 | 3.0(-11) | 4.7(-11) | 7.1(-11) | 8.7(-11) | 9.8(-11) | 1.1(-10) |
| 6 | 4 | 1.3(-10) | 1.3(-10) | 1.4(-10) | 1.4(-10) | 1.5(-10) | 1.5(-10) |
| 6 | 5 | 3.2(-11) | 4.3(-11) | 6.2(-11) | 7.7(-11) | 8.9(-11) | 1.0(-10) |

balance, which yields

$$q(J'\rightarrow J)=\frac{2J+1}{2J'+1}q(J\rightarrow J')\exp[-\Delta E(J,J')/kT]$$

where $E(J,J')>0$ is the energy difference of the two rotational levels, $J>J'$.

## 3 Comparison with previous calculations

In Table 3, we make a limited comparison of our own rate coefficient calculations for *para*-$H_2$ with those of Green & Thaddeus (1976). The latter authors used a scaled CO–He interaction potential, derived from the electron gas model, together with appropriate asymptotic forms, to describe the CO–*para*-$H_2$ ($j=0$) potential. They employed the quantum mechanical CC formalism to evaluate the rotational excitation cross-section, a B5 basis for the CO being used throughout the energy range considered.

**Table 3.** A comparison of rate coefficients for collisional de-excitation, $q(J\rightarrow 0)$, in units of $10^{-10}\,cm^3\,s^{-1}$. Upper entry: present calculations; lower entry (in parentheses): Green & Thaddeus (1976).

| J | T(K) | | |
|---|---|---|---|
| | 10 | 40 | 100 |
| 1 | 0.2328 | 0.3296 | 0.5030 |
| | (0.1757) | (0.3449) | (0.3725) |
| 2 | 0.3519 | 0.4246 | 0.4678 |
| | (0.2764) | (0.3334) | (0.4007) |
| 3 | 0.0278 | 0.0494 | 0.0716 |
| | (0.0439 | (0.0557) | (0.0666) |
| 4 | 0.0384 | 0.0567 | 0.0685 |
| | (0.0262) | (0.0400) | (0.0573) |
| 5 | 0.0062 | 0.0104 | 0.0200 |
| | (0.0040) | (0.0100) | (0.0321) |

The overall agreement with the results of Green & Thaddeus (1976) may be considered to be satisfactory, in view of the uncertainties in the calculations of the potential energy surfaces. We note that, at low temperatures, $q(1\rightarrow 0)<q(2\rightarrow 0)$ according to the results of both calculations.

The interpretation of the observations of far-infrared rotational lines of CO requires rate coefficients for transitions between levels of high $J$ to be evaluated at high temperatures. The CC method is computationally intractable under these circumstances, and the much simpler 'infinite order sudden' (IOS) approximation has been applied to this problem (McKee *et al.* 1982). The system actually studied by these authors was CO–He, using the *ab initio* potential of Thomas *et al.* (1980). McKee *et al.* suggest that the rate coefficients for transitions excited by *para*-$H_2$ should be obtained by scaling the CO–He results according to the ratio of the velocities of He and $H_2$ at a given collision energy, i.e. by a factor 1.37. In Table 4, we compare the results of our own calculations for *para*-$H_2$ at the highest temperature which we considered, $T=250\,K$, with those tabulated by McKee *et al.*, scaled by the factor 1.37. Agreement is worst for the $2\rightarrow 0$ and $4\rightarrow 0$ transitions, improves for intermediate values of $J$ and then deteriorates for the largest values of $J$ that we studied.

**Table 4.** A comparison of rate coefficients, $q(J\rightarrow 0)$, for the rotational de-excitation of CO by *para*-$H_2$, in units of $cm^3 s^{-1}$ and at a kinetic temperature of $T=250$ K (a) present calculations; (b) calculations of McKee *et al.* (1982). Numbers in parentheses are powers of 10.

| J | (a) | (b) |
|---|---|---|
| 1 | 5.82(-11) | 3.16(-11) |
| 2 | 5.12(-11) | 1.75(-11) |
| 3 | 1.02(-11) | 1.01(-11) |
| 4 | 8.12(-12) | 3.96(-12) |
| 5 | 4.19(-12) | 4.21(-12) |
| 6 | 2.12(-12) | 1.81(-12) |
| 7 | 1.59(-12) | 1.58(-12) |
| 8 | 8.57(-13) | 8.93(-13) |
| 9 | 6.01(-13) | 6.67(-13) |
| 10 | 3.63(-13) | 4.41(-13) |
| 11 | 2.20(-13) | 3.21(-13) |

The discrepancies for the $2\rightarrow 0$ and $4\rightarrow 0$ transitions are attributable to differences in the potential energy surfaces employed in the two calculations and not to the dynamical (IOS) approximation, which is most accurate for small $J$ (*cf.* Thomas *et al.* 1980). The IOS approximation is intrinsically less accurate for large $J$, but it should be borne in mind that the accuracy of our own calculations also deteriorates as $J$ increases, for the reasons given in Section 2 above.

## 4 Conclusions

We have presented the results of calculations of rate coefficients for the rotational excitation of CO by *para*- and *ortho*-$H_2$. Reasonable agreement is obtained with earlier calculations by Green & Thaddeus (1976) for *para*-$H_2$ at low temperatures ($T\leqslant 100$ K). Larger discrepancies with the results of McKee *et al* (1982) at higher temperatures are attributable to differences in the potential energy surfaces employed, that of McKee *et al.* being for the CO–He system. It would be informative to compare the rate coefficients reported here with values derived from the more recent CO–$H_2$ potential energy surface of Schinke *et al.* (1984).

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## References

Andres, J., Buck, U., Meyer, H. & Launay, J. M., 1982. *J. Chem. Phys.*, **76,** 1417.
Brechignac, Ph., Picard-Bersellini, A., Charneau, R. & Launay, J. M., 1980. *Chem. Phys.*, **53,** 165.
Flower, D. R., Launay, J. M., Kochanski, E. & Prissette, J., 1979. *Chem. Phys.*, **37,** 355.
Flower, D. R. & Watt, G. D., 1984. *Mon. Not. R. astr. Soc.*, **209,** 25.
Green, S. & Thaddeus, P., 1976. *Astrophys. J.*, **205,** 766.
Green, S. & Chapman, S., 1978. *Astrophys. J. Suppl.*, **37,** 169.
Herzberg, G., 1950. *Spectra of Diatomic Molecules*, Van Nostrand, Princeton, NJ.
Launay, J. M., 1977. *J. Phys. B: Atom. Mol. Phys.*, **10,** 3665.
McKee, C. F., Storey, J. W. V., Watson, D. M. & Green, S., 1982. *Astrophys. J.*, **259,** 647.
Picard-Bersellini, A., Charneau, R. & Brechignac, Ph., 1983. *J. Chem. Phys.*, **78,** 5900.
Prissette, J., Kochanski, E. & Flower, D. R., 1978. *Chem. Phys.*, **27,** 373.
Schinke, R., Meyer, H., Buck, U. & Diercksen, G. H. F., 1984. *J. Chem. Phys.*, **80,** 5518.
Thomas, L. D., Kraemer, W. P. & Diercksen, G. H. F., 1980. *Chem. Phys.*, **51,** 131.