

Rotational excitation of CO in a cool, mixed atomic and molecular hydrogen gas

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ABSTRACT

Context. Rate constants for rotational excitation of CO by atomic hydrogen have recently been recalculated and found to be much larger than was previously believed, larger even than for excitation by H₂.

Aims. To clarify the effect upon CO rotational excitation of an admixture of atomic hydrogen in diffuse molecule-bearing gas.

Methods. The equations of statistical equilibrium in the CO rotation ladder are solved under a variety of conditions typical of CO-bearing gas in the diffuse ISM.

Results. Atomic hydrogen, if present, substantially increases the brightness and excitation temperatures of the CO rotational transitions, and increases the $J = 2-1/J = 1-0$, $J = 3-2/J = 2-1$, etc. line brightness ratios. A modest admixture of atomic hydrogen mimics a pure H₂-gas of substantially higher ambient thermal pressure.

Conclusions. Rotational excitation of CO by atomic hydrogen is important if even a few percent of the hydrogen is in atomic form.

Key words. molecular processes – radio lines: ISM – ISM: atoms – ISM: molecules – ISM: clouds

1. Introduction

Carbon monoxide is observed in absorption in the nearby interstellar medium (ISM) at ultraviolet (Federman et al. 1994), near IR (McCall et al. 2002; Oka et al. 2005) and mm-wavelengths (Liszt & Lucas 1998) and in emission at mm-wavelengths. From the weakest lines detected in the ultraviolet, where $N(\text{CO}) = 10^{12} \text{ cm}^{-2}$, to the Orion nebula where $N(\text{CO}) = 2 \times 10^{19} \text{ cm}^{-2}$ (Liszt et al. 1974), CO is observed over a range of column densities and conditions second only to atomic or molecular hydrogen.

CO rotational emission is the main surrogate for H₂ and the most commonly used marker of “molecular” gas: the assumption is commonly made that, when CO emission is present, the ambient gas is one in which the hydrogen is in molecular form. However, for the diffuse ISM, toward the lower end of the observed range of $N(\text{CO})$, the assumption of a purely molecular gas is less obviously correct, even though CO emission may be much stronger than is generally appreciated. The strength of CO emission rises above the level 0.1 K at $N(\text{CO}) \approx 10^{14} \text{ cm}^{-2}$ and $J = 1-0$ lines at the level of 3–4 K commonly arise from regions of relatively modest line opacity when $N(\text{CO}) < 1-3 \times 10^{16} \text{ cm}^{-2}$ is very small compared to the amount of free gas phase carbon expected for $A_V = 1 \text{ mag}$ (i.e. $3 \times 10^{17} \text{ cm}^{-2}$) (Liszt & Lucas 1998). CO emission as bright as 8–10 K is seen in the immediate vicinity of ζ Oph (Liszt & Lucas 1994; Liszt 1997; Tachihara et al. 2000) even though the line of sight reddening remains below 0.4 mag according to the prescription of Schlegel et al. (1998).

Since the work of Green & Thaddeus (1976), who found that the per-particle rotational excitation of CO was much smaller for hydrogen atoms than for H₂, it has been generally assumed that rotational excitation of CO by atomic hydrogen is

negligible even in diffuse gas which might not be fully molecular. At the densities of molecular hydrogen presumably needed chemically to support a column of CO which is visible in emission, the H₂/H ratio would be large enough to provide whatever excitation is found in the emitting CO. For cases in which the calculated excitation by H₂ is deemed to be insufficient, Wannier et al. (1997) ingeniously suggested that scattering of radiation emanating from nearby dark clouds would provide excitation radiatively, and this suggestion was recently adopted by Bensch (2006) to explain the persistence of CO emission out into the diffuse halo of the dark cloud B5, in contrast to C I, whose emission is confined to the dark regions.

An intimation that excitation by H-atoms would prove important is found in the work of Chu & Dalgarno (1975), who calculated H-CO excitation rates which were larger – in some cases order of magnitude larger – than those of Green & Thaddeus (1976). Indeed, the recent scattering calculations of Balakrishnan et al. (2002, BYD) which use a highly-refined ab initio H-CO interaction potential, show that the per-particle rates for rotational excitation of CO by H-atoms are much larger than calculated even by Chu & Dalgarno (1975), and larger for H-atoms than for either H₂ or He. In this case the excitation of CO by atomic hydrogen in diffuse gas really cannot be neglected and the thermal pressure of diffuse gas cannot be inferred from calculation of the CO excitation temperatures assuming pure H₂, as has been done previously (Liszt & Lucas 1998).

In light of this recent change, this paper considers the effects of various cool, mixed atomic and molecular hydrogen gases upon the rotational excitation of CO. In Sect. 2 we assemble the relevant excitation rates and discuss, briefly, the means we have used to calculate the rotational excitation of CO in diffuse gas. In Sect. 3 we show the results of these excitation calculations.

2. Collisional excitation of CO

2.1. Collision rates and collision partners

The chief collision partners for CO are hydrogen atoms, for which collision rates were recently calculated by BYD, ortho- and para- H_2 (Flower 2001) and helium (Cecchi-Pestellini et al. 2002); we have included excitation by electrons (Dickinson & Munoz 1977) but this is a very minor effect because CO has such a small permanent dipole moment (0.112 Debye). However, this small dipole moment is responsible for many of the excitation effects discussed here, principally because it renders the excitation sensitive to the ambient thermal pressure (as opposed say, to the density) in a pure H_2 gas. This situation changes drastically for excitation by atomic hydrogen, as shown below. It is often the case that the Green-Thaddeus rate constants are approximated by the expressions given by Warin et al. (1996). We have followed that practice in this work as well when comparisons between the old and new excitation rates are made.

We assume the standard ratio $[\text{He}]/[\text{H}] = 0.086$ and take $n(e)/n(\text{H}) = 2 \times 10^{-4}$, typical of diffuse gas; although electrons do not provide significant excitation for CO they are almost solely responsible for HCO^+ emission from diffuse gas, however weak it may be (Liszt & Lucas 1994; Lucas & Liszt 1996). We assume that the ortho/para ratio in H_2 is 3 and that the ortho- and para- ladders are thermalized by spin exchange with protons (Black & Dalgarno 1977); this assumption provides the means whereby the kinetic temperatures of diffuse H_2 -bearing regions are inferred. The calculations performed here undoubtedly extend somewhat beyond the range where the gas might be expected to host electron and proton fractions as large as 10^{-4} but we will demure from drawing conclusions which are prejudiced in this way.

The extent to which the new BYD excitation rates per particle are so much increased, and so much greater for H-atoms than for H_2 , is shown in Fig. 1. There, for a range of temperatures, we have plotted the sum of all excitation rates out of the $J = 0$ rotational level as a function of the molecular fraction, at a fixed total thermal pressure; the pressure is summed over all the particles which are the chief CO collision partners. Note that, for a fully molecular gas, the plotted total rate is nearly the same for $T_K = 10\text{--}100$ K: it varies with pressure, only, indicating that the rate constants themselves vary in such a way as to counteract the decline of density with T_K at fixed pressure. By contrast, the total rates in the atomic gas vary much more strongly with temperature, declining by a factor 4 from 10 to 100 K, although they are always substantially larger than for H_2 at each value of T_K . The dashed (red) line at the bottom in Fig. 1, representing the same calculation performed with the rate constants of Green & Thaddeus (1976) at 40 K, shows just how drastic a revision of the excitation scheme the new rate calculations of BYD imply.

2.2. Line brightnesses

For a gas of molecules having excitation temperature T_{exc} , emitting at frequency ν with optical depth τ across the medium, the brightness of a line above the cosmic microwave background at frequency ν is

$$T_B = (1 - \exp(-\tau))[J(T_{\text{exc}}) - J(T_{\text{cmb}})] \quad (1)$$

where $J(x) = (h\nu/k)/(\exp(h\nu/kx) - 1)$, and h and k are the Planck and Boltzmann constants. For the $J = 1\text{--}0$ line of CO at 115.271 GHz, $J(x) - J(T_{\text{cmb}}) \rightarrow x - 3.5$ K for $x \gg T_{\text{cmb}}$ while for $J = 2\text{--}1$ at two times higher frequency the brightness deficit is approximately twice as large (6.5 K).

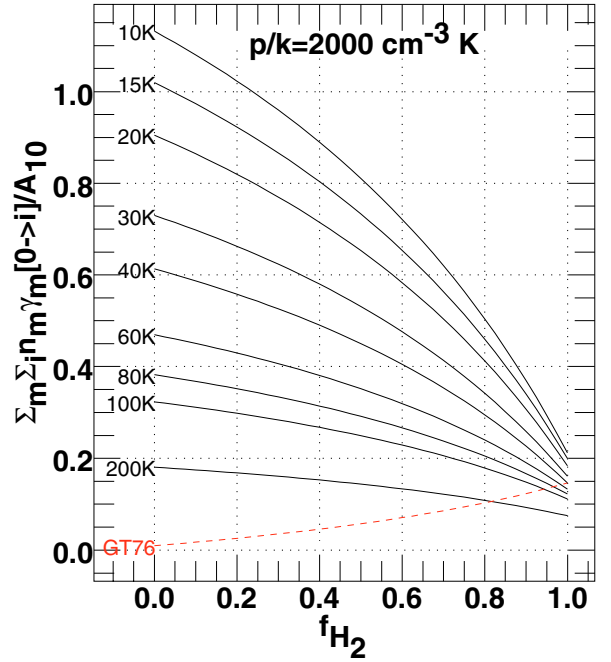


Fig. 1. The total upward collision rate out of the $J = 0$ level of CO in an ambient gas having $p/k = 2000 \text{ cm}^{-3} \text{ K}$, normalized by the spontaneous emission coefficient of the $J = 1\text{--}0$ transition $A_{10} = 7.2 \times 10^{-8} \text{ s}^{-1}$, for varying kinetic temperature and fractions f_{H_2} of H-nuclei in H_2 . The rates $n_m \gamma_m [0 \rightarrow i]$ for $J = 0\text{--}i$ transitions have been summed over all species m ($m = \text{H-atoms, He, H}_2$ and electrons) and higher-lying levels $i > 0$. The dashed (red) line at bottom is the result for 40 K using Warin et al. (1996)'s approximations to the atomic hydrogen–CO excitation rates of Green & Thaddeus (1976).

Figure 2 shows $J(T_{\text{exc}}) - J(T_{\text{cmb}})$ for the $J = 1\text{--}0$ CO line over the same range of conditions as in Fig. 1, after solution of the equations of statistical equilibrium in the limit of zero CO column density. Again we see that for a purely molecular gas, the $J = 1\text{--}0$ excitation is nearly the same, regardless of the temperature while, for the atomic gas and the BYD excitation rates, the maximum brightness increases with T_K up to 20 K, and then declines strongly as T_K increases further. However, for all molecular fractions, the CO line is much more highly excited in a more nearly atomic gas with the new rates.

At bottom in Fig. 2 we see that the ratio of brightnesses in the two lowest-lying CO lines (calculated in the limit of zero column density) is dependent on the pressure alone in a pure H_2 gas, as long as $T_K > 15$ K. The excitation supplied by hydrogen atoms is strongly temperature sensitive (at this fixed pressure) but produces a uniformly higher ratio of $J = 2\text{--}1$ to $J = 1\text{--}0$ brightnesses and a higher ratio of optical depths in the two lines in the same sense as long as $T_K \lesssim 100$ K.

3. Rotational excitation of CO in a cool, mixed atomic and molecular hydrogen gas

Figure 3 shows the result of a series of excitation calculations performed using an LVG code for $N(\text{CO})/\Delta V = 2 \times 10^{15} \text{ cm}^{-2} (\text{km s}^{-1})^{-1}$ and the new CO excitation rates of BYD. The fraction of H-nuclei in H_2 varies from 0.25 at left to 1 in the rightmost column, in steps of 0.25. The row at top shows $J(T_{\text{exc}}) - J(T_{\text{cmb}})$ for the $J = 1\text{--}0$ line; in the middle is the brightness temperature of the $J = 1\text{--}0$ line, $T_B(1\text{--}0)$, and at bottom the ratio $T_B(2\text{--}1)/T_B(1\text{--}0)$ is shown. The optical depth at any point

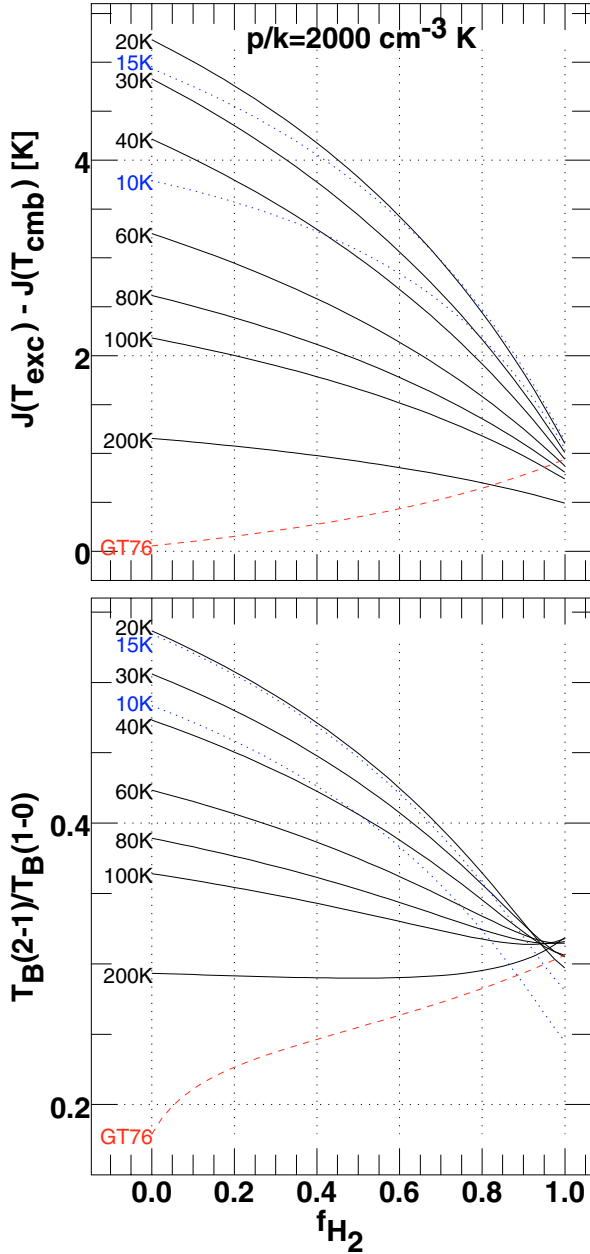


Fig. 2. Rotational excitation calculations for CO in ambient gases of varying proportions of hydrogen atoms and molecules for temperatures in the range 10–200 K, in the limit of zero CO column density. At top is shown the bracketed quantity in Eq. (1), the limiting brightness of the $J = 1-0$ line. At bottom the ratio of brightnesses in the $J = 2-1$ and $J = 1-0$ lines is plotted. The dashed (red) lines are results for 40 K using the Warin et al. (1996) approximations to the results of Green & Thaddeus (1976).

may be gauged by comparing the top two rows, whose ratio at any point is $(1 - \exp(-\tau))$.

Reflecting the strong dependence on pressure, contour lines in the top two panels in Fig. 3 are predominantly vertical, at least when the $J = 1-0$ transition is far from being thermalized by collisions (i.e. except at the very lower right corner of each panel). Contours in the gases dominated by atomic hydrogen have substantially more curvature but run predominantly vertical nonetheless; this belies their strong temperature sensitivity, seen in Figs. 1, 2.

The quantity $J(T_{\text{exc}}) - J(T_{\text{cmb}})$ plotted in the top panel is the one most generally affected by an admixture of atomic hydrogen; an atomic gas fraction of 25% may double this measure of the excitation over much of region mapped (see also Fig. 2 at top). Effects on $T_B(1-0)$ are quite pronounced for weaker lines – $T_B(1-0)$ doubles for even a 25% admixture of atoms when the line brightness is below 1 K, while the brightness temperature ratio in the lowest row varies little. For brighter lines having $T_B(1-0) > 1$ K, increased excitation begins to redistribute population into the higher J -levels and the line ratio in the bottom row varies somewhat more. For instance, at $\log p/k = 3$, $\log T_K = 1.5$, a 25% admixture of atomic hydrogen produces a higher line brightness ratio which corresponds to a tripling or quadrupling of the pressure in a pure H_2 gas.

3.1. Comparison with older rate constants

The disparity between use of the new (BYD) and old (Green & Thaddeus 1976) rates for CO rotational excitation by H-atoms may be gauged by comparing Figs. 3 with 4, where the calculation is repeated using the excitation rates of Green & Thaddeus (1976). For a gas composed of 75% atomic hydrogen, at $\log p/k = 3$ and $\log T_K = 1.5$, the $J = 1-0$ line brightnesses are 0.2 using the rates of Green & Thaddeus (1976) and 1.5 K with those of BYD. The change in the line brightness ratio is numerically smaller, but corresponds to substantial difference in the pressure of a fully molecular gas.

3.2. Radiative or collisional excitation?

Wannier et al. (1997) suggested that, in diffuse clouds, scattering of incident line radiation emanating from external dark clouds could be a stronger source of CO rotational excitation than collisions with the host hydrogen gas. In part, this was motivated by the weakness of the excitation attributed to atomic hydrogen by Green & Thaddeus (1976), as illustrated by the arguments of Bensch (2006) regarding the detectability of CO emission in the halo of B5, quoting the older rates of (Green & Thaddeus 1976, his Sect. 5.2). Given that the $N(\text{CI})/N(\text{CO})$ ratio increases into the halo or B5, the more extended distribution of CO emission must be explained somehow.

In the halo of B5, the brightnesses of the $J = 1-0$ and $2-1$ lines of ^{12}CO are given as 1.6 K and 0.9 K, respectively, at the first position outside the body of the cloud where CI is not detected (Fig. 2 and Table 2 of Bensch 2006). Figures 1 and 2 here show that a mixed gas of typical thermal pressure $p/k = 2 \times 10^3 \text{ cm}^{-3} \text{ K}$, like that inferred for the halo of B5 by Wannier et al. (1999), can provide excitation comparable to that observed in the halo of B5 if the newer excitation rates are employed, even in the small optical depth limit. Excitation calculations using the older rates cannot approach the observed levels of excitation as Bensch (2006) indicated.

CO emission in the near halo of B5 is apparently quite optically thick, because the $^{12}\text{CO } J = 1-0$ line is only six times as bright as that of ^{13}CO . Resonant scattering constitutes an additional source of support for rotational excitation (Leung & Liszt 1976) but it creates a potential problem in invoking the radiative scattering mechanism of Wannier et al. (1997) to explain the observed excitation in the halo of a dark cloud. A halo molecule which is separated by an optically thick, pure scattering atmosphere from the supposed bright surface of the cloud may receive a flux which is severely attenuated by multiple scattering in the intervening medium.

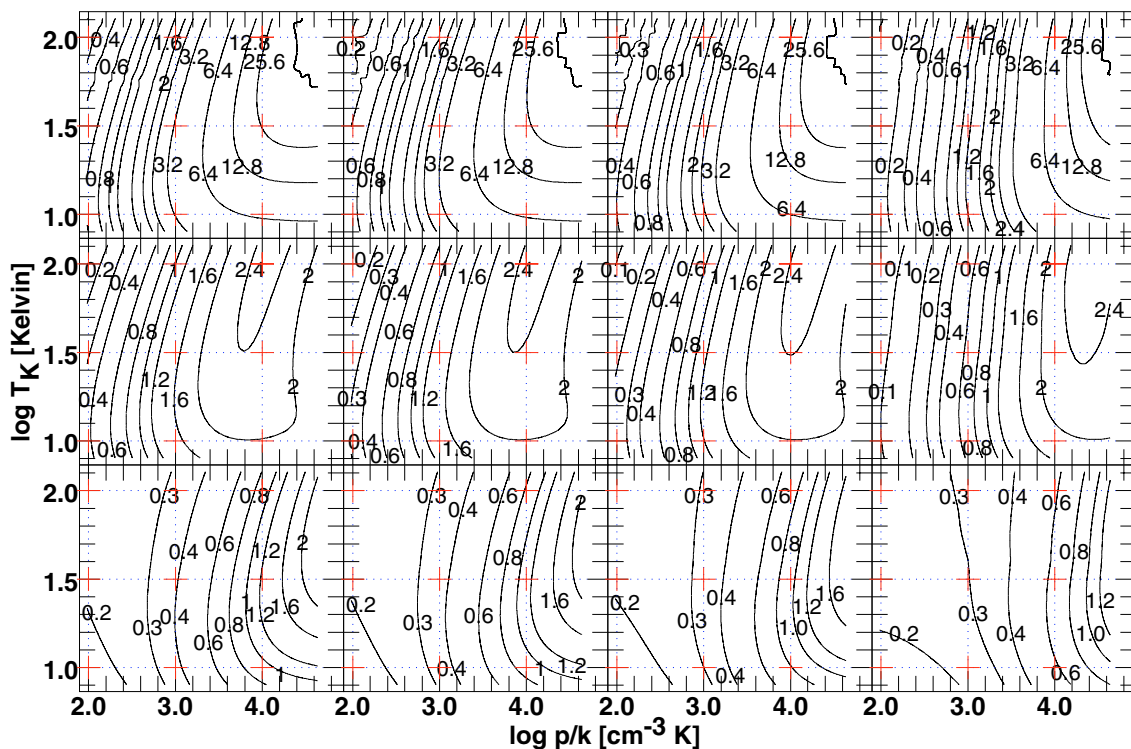


Fig. 3. Rotational excitation calculations for CO in ambient gases having differing proportions of hydrogen atoms and molecules, using the excitation rates for excitation of CO by H-atoms recently calculated by Balakrishnan et al. (2002). From left to right in each column the fraction of H-nuclei in H_2 varies from 0.25 to 1 in steps of 0.25. The row at top shows $J(T_{exc}) - J(T_{cmb})$ for the $J = 1-0$ line; in the middle is the brightness temperature of the $J = 1-0$ line, $T_B(1-0)$, and at bottom the ratio $T_B(2-1)/T_B(1-0)$ is shown. The calculations were done using an LVG code with $N(CO)/\Delta V = 2 \times 10^{15} \text{ cm}^{-2} (\text{km s}^{-1})^{-1}$. Contours are shown at levels 0.1, 0.2, 0.3, 0.4, 0.6, 1, 1.2, 1.6, 2, 2.4, 3.2, 6.4, 12.8 and 25.6 in appropriate units in each panel.

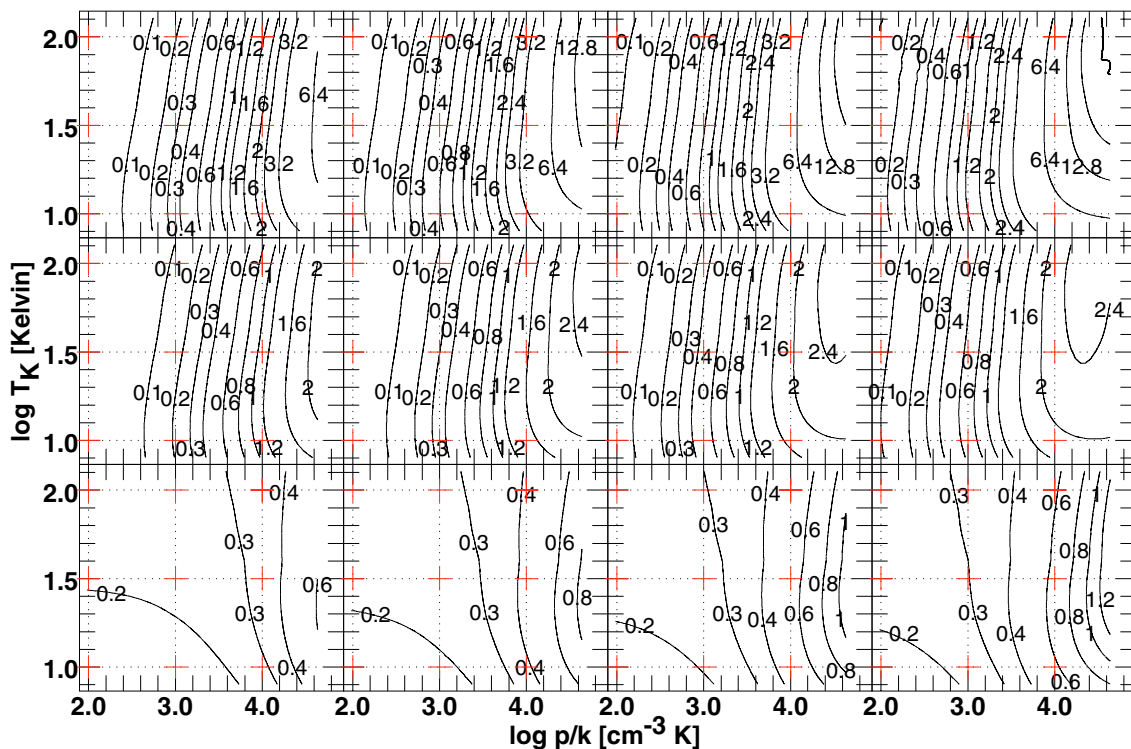


Fig. 4. As in Fig. 3, but using the approximation of Warin et al. (1996) to represent the much smaller values of CO rotational excitation by atomic hydrogen calculated by Green & Thaddeus (1976).

3.3. Higher-lying CO transitions

Although not discussed explicitly here, it is obvious that the new, larger excitation rates of BYD will act to brighten the $J = 3-2$ and higher-lying CO lines relative to calculations with older rates or gases considered purely molecular. van Dishoeck et al. (1991) observed the $J = 3-2$ line in translucent and high-latitude clouds. Although the line was not detected toward ζ Oph, they did find that excitation calculations based on the $J = 3-2$ line of ^{12}CO implied densities which were much higher than given by other diagnostics. Like others, van Dishoeck et al. (1991) did not include excitation by H-atoms, but they noted that use of the Chu & Dalgarno (1975) rates would have had a modest effect. It is possible that a reexamination of these observations using the BYD rates would alleviate this discrepancy.

4. Summary of considerations

Rotational excitation of CO by atomic hydrogen has generally been considered to be negligible, following the results of Green & Thaddeus (1976). However the much-larger rates for rotational excitation of CO by atomic hydrogen recently calculated by Balakrishnan et al. (2002), larger for H-atoms than for H_2 , imply a much higher level of excitation for CO in any gas which is less than fully-molecular, diffuse or otherwise: excitation calculations should include the contribution of atomic hydrogen whenever there is reason to believe that the CO-bearing gas is more than a few percent atomic.

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