THE ASTROPHYSICAL JOURNAL, 366:277–285, 1991 January 1

CO FUNDAMENTAL BANDS IN LATE-TYPE STARS. II. SPECTRUM SIMULATIONS FOR F–K STARS

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Received 1989 December 29; accepted 1990 June 29

ABSTRACT

This paper is a continuation of our study of the carbon monoxide vibration-rotation bands in late-type stars. The $\Delta v = 1$ fundamental transitions of CO near 4.6 μm can be used as probes for the thermal structure of the upper atmospheres of cool stars, where observations using different spectral diagnostics recently have led to contradicting results: the chromospheric temperature rise, deduced from UV/visual line observations, cannot be reconciled with temperature profiles inferred from infrared molecular line observations. A possible solution to this dilemma is the "thermal bifurcation" scenario, where cool and warm areas co-exist at a given altitude in the upper atmosphere. The cool areas, controlled by radiative equilibrium dominated by the CO $\Delta v = 1$ bands, are responsible for the observed, strong molecular absorption spectra; whereas the hot non-radiatively heated, "chromospheric" areas are observed predominantly in high-temperature UV/visual atomic lines. In the two-component model any observed spectrum is an average over the inhomogeneous stellar surface, and need not be representative of either component. The parameters of the empirical models can depend rather crucially on the spatial averaging properties of the observed species.

In this investigation we focus on the cool, molecular atmospheric component. We apply a non–LTE spectrum synthesis code for stellar atmospheres between spectral types F5 and K5 in order to establish the CO fundamental bands as a diagnostic tool. Spectra computed with varying stellar parameters reveal the sensitivity of the CO spectra to these parameters. The strong lines in CO $\Delta v = 1$ spectra are affected by elemental abundances and surface gravity but cannot be used easily to derive these properties. On the other hand, CO line intensities respond strongly to the thermal structure of the upper atmosphere and thus are sensitive temperature probes, even if the excitation of the bands deviates from local thermodynamic equilibrium. We examine the impact of non–LTE effects on CO spectra quantitatively, including errors introduced by uncertainties in the crucial cross sections for vibrational excitation of CO through atomic hydrogen.

Our study demonstrates that the CO $\Delta v = 1$ bands are valid probes for the temperature structure over a broad range of physical conditions and thus can contribute fundamentally to the study of the outer atmospheres of stars of late spectral type.

Subject headings: infrared: spectra — molecular processes — stars: atmospheres — stars: late-type

I. INTRODUCTION

The infrared (IR) vibration-rotation bands of carbon monoxide have long been recognized as important spectral diagnostics for cool stellar atmospheres (e.g., Hall 1970). CO is the most abundant molecule (exceeded only by H_2 in very cool stars) owing to the high elemental abundances of its constituents and its large binding energy. CO has many infrared transitions originating from a wide range of excitation states. The corresponding lines form over a broad altitude range and are useful in studies ranging from convection dynamics in the deeper layers of stellar atmospheres to cool winds in the outermost layers (Ridgway and Friel 1981). In addition, CO lines are abundance tracers for atomic oxygen and carbon (Tsuji 1986). Determination of isotopic abundances (^{13}C, ^{17}O, ^{18}O) is essential in studies of the evolutionary status of late-type giants (Harris, Lambert, and Smith 1988).

Most previous studies have used the $\Delta v = 2$ overtone lines of CO at 2.3 μm, and higher overtones in the near-IR, which are much more accessible from a technical standpoint than the $\Delta v = 1$ fundamental bands near 4.6 μm. Furthermore, the overtone lines are weaker than the fundamental bands and therefore form deeper in the stellar atmosphere, where LTE generally is valid and line saturation is less a problem in abundance studies. However, the fundamental lines ($\Delta v = 1$) are of particular interest in the study of the higher atmospheric layers. The strongest $\Delta v = 1$ lines form at or above the temperature minimum in "chromospheric" solar and stellar models. Earlier studies of the Sun by Ayres and Testerman (1981) and Arcturus by Heasley *et al.* (1978) revealed that observed CO spectra cannot be reconciled with homogeneous chromospheric models inferred from observations in the visible and ultraviolet, e.g., by Vernazza *et al.* (1981) and Ayres and Linsky (1975, hereafter AL). Although previous studies clearly indicated the importance of including CO observations in the modeling of (the apparently inhomogeneous) stellar atmospheres, quantitative analysis of Arcturus-type spectra has been limited by the uncertain magnitude of non–LTE effects in the formation of the $\Delta v = 1$ bands in the cool, low-gravity stars.

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We have begun a new study of cool stellar atmospheres based on the measurement and analysis of CO fundamental spectra. The observational part of our study has been triggered by recent advances in instrumentation for IR spectroscopy (Wiedemann *et al.* 1989). In parallel, we developed a straightforward formalism to treat departures from LTE in the CO $\Delta v = 1$ bands of cool stellar atmospheres (Ayres and Wiedemann 1989, hereafter Paper I). The numerical spectrum synthesis procedure permits a more accurate interpretation of observed CO spectra.

In the present work we apply the procedure of Paper I to a range of stellar atmosphere models to study the CO $\Delta v = 1$ spectrum and establish its use as a remote sensor of thermal conditions in late-type stars. We compute spectra for a series of radiative-equilibrium (RE) and semi-empirical chromospheric models to examine the sensitivity of CO $\Delta v = 1$ bands to several stellar parameters and assess the errors in spectrum interpretation due to insufficient knowledge of these properties. The largest uncertainty in the interpretation of low-gravity red giant spectra has usually been the cross sections for vibrational excitation of CO by atomic hydrogen collisions: these determine the magnitude of "non–LTE line darkening" which can mimic a high-altitude depression in the thermal profile. We examine quantitatively the influence of the residual uncertainties in the recently published laboratory measurements of the CO-H collision rates. The present investigation constitutes a basis for a quantitative analysis of observed CO spectra, which we will present separately (Wiedemann *et al.* 1990).

II. NON–LTE SPECTRUM SYNTHESIS CALCULATIONS

a) *Method*

The radiative transfer code used in this investigation computes CO $\Delta v = 1$ spectra for an atmospheric model by solving the statistical equilibrium and radiative transfer equations in the line-forming layers. These equations are strongly and nonlinearly coupled in "classical" non–LTE problems like that of the Ca II H and K lines in the solar chromosphere, where the radiation field dominates the excitation state populations. However, owing to the large CO-H collision rates and small radiative decay rates, the CO fundamental bands are much closer to LTE in normal cool stellar atmospheres. The statistical equilibrium and radiative transfer equations are only weakly coupled and can be solved by "Λ-iteration" (Mihalas 1978, § 6-1): given an initially assumed state distribution (e.g., a Boltzmann distribution) at all levels of the atmosphere, the radiation field is computed by the formal solution of the radiative transfer equation. That radiation field establishes a new excitation state distribution through the statistical equilibrium relations. The iteration cycle is repeated until the populations and radiation fields are self-consistent. In the "classical" non–LTE problem in stellar atmospheres (Mihalas 1978), the Λ-iteration is impractical because the strong, nonlinear coupling requires a prohibitively large number of iterations to obtain convergence. On the other hand, the partial-linearization techniques developed for atomic and ionic lines (e.g., Auer and Heasley 1976) cannot be applied directly to the CO problem because of the enormous number of bound states and transitions involved: the timing of the linearization technique scales typically with the third power of the number of transitions. The Λ-iteration is successful because it scales in direct proportion to the number of transitions. Furthermore, the density of atomic hydrogen, the most important collision partner for CO, increases exponentially inward in normal stellar atmospheres. This guarantees thermalization of the radiation field within a few optical depths of the $\tau = 1$ surface, and therefore rapid convergence of the iteration process. No more than about five Λ-iterations were required for a solution of the CO non–LTE problem in a cool star atmosphere with $\log g > 0$. In practice, the calculation is performed twice to allow for the different abundances of the majority species $^{12}C^{16}O$ and $^{13}C^{16}O$. Although $^{12}C^{18}O$ lines are very strong in some evolved low-gravity stars, we restricted the non–LTE calculations to $^{12}C^{16}O$ and $^{13}C^{16}O$ for the sake of computational effort. Further details can be found in Paper I.

We synthesized the CO line spectra in the range 2140–2145 cm^{-1}. This interval contains a large number of $\Delta v = 1$, R-transitions ($\Delta j = +1$) from vibrational states up to $v = 6$, and lines from all CO isotopes. It also is the most easily observed spectral window from the ground, since it is largely free of contamination by atmospheric absorption lines. We computed the $\Delta v = 1$ rest frequencies from the Dunham coefficients given by Guelachvili *et al.* (1983), and adopted the oscillator strengths of Kirby-Docken and Liu (1978), which are consistent with the Einstein coefficients for spontaneous emission A_{ij} published by Radzig and Smirnow (1985).

For comparison, an LTE spectrum is produced during each run of the numerical simulation. The LTE spectrum is obtained by setting the CO departure coefficients (state population densities divided by their LTE value) equal to unity, forcing a Boltzmann distribution for the vibrational states. Thus LTE and non–LTE spectra are created in an entirely consistent manner. The LTE spectra produced by the non–LTE Λ-iteration code differ slightly from those generated by a specialized LTE spectrum synthesis program also used in the present study. One can find discrepancies in line intensities of a few percent in weak lines formed deep in the atmosphere, where the temperature increases rapidly with the mass column density m. These discrepancies are due to simplifying numerical approximations made in the Λ-iteration code; for example, the CO energy spectrum is parameterized as that of a pure harmonic oscillator and pure rigid rotor, which leads to economies in the specification of the rate equations. In the specialized LTE code the correct, laboratory-derived term values are used. The small magnitude of the resulting differences supports the accuracy of the approximations in the non–LTE code. However, in modeling the hotter, high-density stars and the weaker lines in cool stars, the simpler and more accurate LTE code is preferable.

In addition to contrasting the shapes of individual spectral lines, non–LTE effects in CO lines can be illustrated by comparing the source function $S(\tau)$, (ratio of total emissivity and absorptivity) to the local Planck-function $B_\nu(T)$ (the LTE source function) in the line-forming region. The source function $S(\tau)$ contains a contribution from the Planck function, representing local thermal emissions at optical depth τ, and a scattering term arising from the re-emission of photons absorbed from the ambient radiation field J_ν, the latter usually representative of excitation conditions in much deeper layers. Scattering in CO $\Delta v = 1$ lines is noncoherent due to rapid collision—induced rotational transitions within a vibrational excitation state. Schematically, the relative importance of B compared with J in the source function is controlled by the factor $\varepsilon = c_{ij}/A_{ij}$ ("collisional epsilon"), the ratio of collisional de-excitations (thermal quenching) to spontaneous radiative decays. If collisions dominate the excitation–de-excitation

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equilibrium in the line-forming region ($0.3 < \tau < 3$), the emerging radiation field will be purely thermal and reflect the Boltzmann distribution of excited states at the $\tau \sim 1$ kinetic temperature. If radiative rates dominate collisions, the local vibrational state distribution (at optical depth τ), is controlled by radiation fields formed deeper in the stellar atmosphere and the excitation state distribution can deviate considerably from a Boltzmann distribution of the local temperature. In the higher layers, above $\tau = 1$, the radiation field can be approximated by a dilute Planck function, $J_\nu \sim \frac{1}{2}B(T_{\rm rad})$, where $T_{\rm rad}$ is characteristic of the thermal conditions in the deeper layers, where the strong CO lines thermalize [$\tau_{\rm th} \sim (\varepsilon + 1)/\varepsilon$]. The IR Planck function scales nearly linearly with temperature in a stellar atmosphere. Thus, if there is no sharp temperature increase toward the photosphere, (as is generally the case for the CO line-forming regions), the radiation field in the line-forming layers will be less than the local blackbody emission; consequently, the source function at $\tau \sim 1$ will be below the Planck function. In that case the $\Delta v = 1$ absorption lines will be deeper than in LTE, and the actual kinetic temperature near $\tau \sim 1$ would be higher than inferred from an LTE analysis of the line depths.

b) CO *Collisional Cross Sections*

The pivotal component of any non–LTE problem is the set of collisional cross sections connecting the radiating states. Previous investigations of non–LTE effects in the CO $\Delta v = 1$ bands (Carbon, Milkey, and Heasley 1976; Hinkle and Lambert 1975) lacked reliable rates for the dominant relaxation mechanism of vibrationally excited CO: collisions with hydrogen atoms (Thompson 1973). Either large deviations from LTE, or essentially none, were found depending on which of two available sets of CO-H cross sections were used. A discussion of collision rates between CO and a number of perturbers, including atomic hydrogen, can be found in Paper I. Here, we adopt the CO-H relaxation times obtained by Glass and Kironde (1982, GK) in a shock-tube experiment, which to our knowledge, is the only experiment to date aimed directly at the determination of CO-H collision rates. In addition, we computed spectra using several alternative collision rates in order to gauge the magnitude of possible errors arising from that source.

c) *Stellar Models*

We use a grid of stellar radiative-equilibrium atmosphere models by Bell *et al.* (1975, hereafter BEGN), discussed in detail by Gustafsson *et al.* (1975); and a number of semi-empirical, chromospheric models from the literature. The BEGN RE models include the effects of molecular line cooling in the outer layers, but treat it in LTE. This gives rise to an inconsistency with the non–LTE spectrum synthesis calculations of our work, to the degree that departure from LTE in CO (the dominating cooling species at high altitudes) affects the temperature structure in the outer layers of the atmosphere. A self-consistent solution requires simultaneous atmospheric structure and spectrum synthesis calculations under non–LTE conditions and is a formidable task. However, the use of the Λ-iteration procedure for the molecular line formation might make a detailed non–LTE treatment more tractable in the atmospheric structure codes. Recent numerical estimates (Ayres 1991) indicate that non–LTE effects in the CO cooling do not affect the temperature structure of the models considered here. Further, the use of powerful statistical "supermultiplet" techniques (Anderson 1989) might even eliminate the necessity to treat the molecular non–LTE problem in quite the detail that it superficially seems to demand.

Our non–LTE calculations indicate that LTE is a good assumption for the CO line formation in the BEGN models with $\log g \geq 1.5$. The departure coefficients deviate from unity mostly in higher layers not treated in the BEGN RE simulations. When non–LTE effects in the CO $\Delta v = 1$ bands are important, then they should *increase* the RE temperature where the CO lines become optically thin, because molecular cooling is maximized in LTE. Conversely, the non–LTE-effects should slightly lower the temperature in the deeper layers, where the CO cooling is depressed in LTE, but permitted to an increasing extent, as the thermalization depth moves inward. Thus, non–LTE effects would tend to smooth out abrupt drops in temperature due to the sudden onset of CO cooling in the LTE regime (see, e.g., Anderson's (1989) RE model of the solar outer atmosphere, which exhibits a ~ 1000 K drop in temperature at the height where the strong $\Delta v = 1$ lines become optically thin).

BEGN caution that their LTE models are unreliable in the highest layers due to insufficient knowledge of opacity sources and their numerical treatment. This introduces additional ambiguities into the CO spectrum calculations for cooler stars where the strongest CO fundamental lines originate in these layers. The strongest CO lines become optically thick even above the top layers of many of the BEGN models. In these cases it was necessary to extend the models (at constant T) outward to $\tau_{\rm CO} \ll 1$. The modifications do not affect the computed continuum flux as $\tau_{5\,\mu{\rm m}} \ll 1$ in those layers. In view of the difficulties cited by BEGN in their comprehensive atmosphere calculations, we made no attempt to verify radiative equilibrium in the extended isothermal layers. Some of the synthetic spectra were computed for oxygen and carbon abundances different from those used to generate the stellar models: abundance variations of the magnitude considered would have very little effect on the atmospheric thermal profile (Gustafsson *et al.* 1975).

The semi-empirical chromospheric models used here were derived from visible or ultraviolet line observations. We extended these models on the photospheric side (with the appropriate BEGN model), if the published thermal profiles did not reach down into the 5 μm continuum-forming layers. The photospheric extrapolation has no effect on the core brightness temperatures of the CO lines, but is necessary to predict the proper residual fluxes ($f_{\rm line}/f_{\rm cont}$) for comparison with Fourier transform spectra without absolute flux calibration

The stellar models were treated in the plane-parallel approximation on a temperature-mass column density $T(m)$ scale, and the RE models are parameterized as ($T_{\rm eff}$, $\log g$, s): g is the surface gravity (cm/s^2), $T_{\rm eff}$ is the effective temperature and s denotes nominal solar abundances (as used by BEGN).

III. SENSITIVITY STUDY

Here, we explore the sensitivity of CO $\Delta v = 1$ spectra to fundamental stellar parameters, beginning with the spectrum of a representative red giant. We then alter the parameters of the reference model and discuss the apparent response of the CO spectrum. By this approach, we can assess the errors introduced into the spectrum interpretation by uncertain input parameters and non–LTE effects.

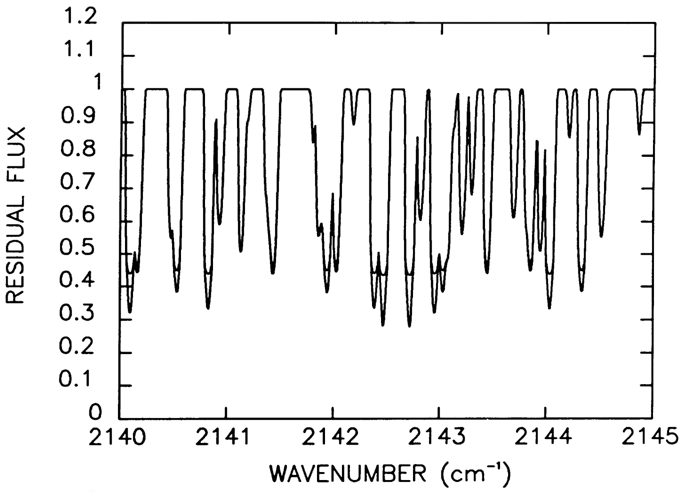

FIG. 1.—CO $\Delta v = 1$ non–LTE spectrum for the reference (4000, 1.5, *s*) model. *Upper spectrum*: LTE; *lower spectrum*: non–LTE.

a) Reference Model

Figure 1 depicts the computed non–LTE spectrum for the (4000, 1.5, *s*) model which serves as a basis for the following discussion. The stellar model is identical to the radiative equilibrium (RE) model of BEGN below $\log m = 0.3$ and we extended it to $\log m = -4.0$ at constant temperature. It represents a low-gravity giant star of spectral type mid-K. Figure 2 illustrates the run of the Planck function $B(T)$, with mass column density. The line-center optical depth τ as a function of m for the strong CO line, 3–2 R14, also is shown. To illustrate the magnitude of non–LTE effects, the source function S for a line from each vibrational state of $^{12}C^{16}O$ is compared to the local Planck function. Figure 2 shows that for all lines up to $v_L = 3$ the respective source function is less than the Planck function at $\tau = 1$, thereby producing a deeper absorption core than in LTE. The effect of the exponential Boltzmann factor, which for higher v forces $\tau = 1$ deeper into the atmosphere, is partially canceled by the increasing A_{ij}'s($\sim v$), resulting in smaller collisional epsilons, i.e., stronger non–LTE darkening.

The lines from higher vibrational states are formed successively deeper in the atmosphere and therefore are progressively less affected by scattering. In the outermost layers ($\log m < -2$) a reversal in the source functions ($S_{v+1} > S_v$) occurs for $v > 2$, due to successively smaller epsilons ($A_{ij} \sim v$, but c_{ij} const.) and to the higher radiation temperatures corresponding to the line forming region at $\tau = 1$. The source function reversal is without consequence, however, as it occurs at shallow optical depths that contribute negligibly to the emergent line intensities.

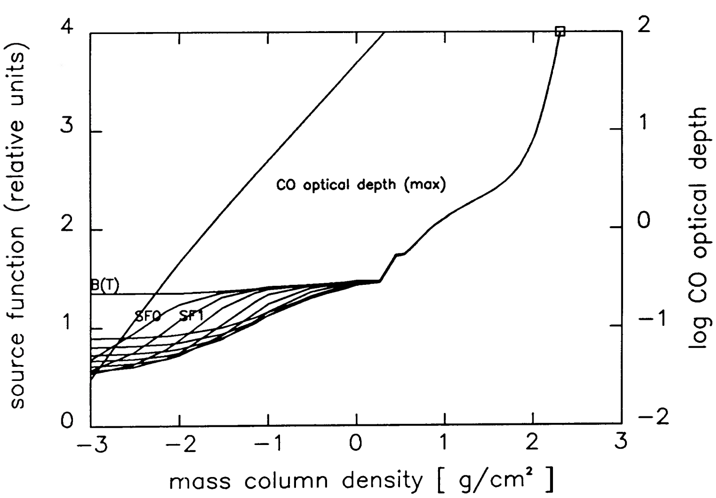

FIG. 2.—Source functions (SF) of the CO lines in the (4000, 1.5, *s*) model and optical depth τ for the strongest line, 3–2 R14 (right scale). $B(T)$: run of blackbody radiation function with mass column density.

b) Effective Temperature and Boundary Temperature

Synthetic spectra for models with effective temperatures from 4000 to 6000 K and low surface gravities are dominated by the temperature sensitivity of the CO abundance. The strong lines in the cooler models become optically thick above the highest layers of the BEGN models in the extrapolated part of the $T(m)$ profile. The CO line cores saturate to the intensity corresponding to the stellar boundary temperature T_b. Accordingly, the appearance (residual intensities) of the strong lines is similar in the cool models with similar ratios of $T_b/T_{\rm eff}$. However, differences arise when the weaker lines are considered. These lines form at lower altitudes where the temperature is a stronger function of m. The onset of CO dissociation above 4000 K rapidly forces ($\tau = 1$) deeper into the atmosphere where the lines respond more strongly to differences in the temperature profiles. In the $T_{\rm eff} = 5500$ K model only the strongest lines reach $\tau = 1$ in the flat part of the $T(m)$ profile, and the saturation effect has almost disappeared. CO is largely dissociated at the temperatures of the 6000 K model and all of the $\Delta v = 1$ lines are form in the photosphere. CO cooling becomes progressively less important in stars with $T_{\rm eff}$ exceeding 5000 K (Johnson 1973), although it apparently is more important than previously indicated in the LTE simulations for stars as hot as the Sun (e.g., Ayres 1981; Anderson 1989). Consequently, CO lines cannot be used as probes for the highest layers of these relatively warm atmospheres. (The Sun itself is an exception, as probing of high-altitude layers is possible through extreme limb observations). The strongest overtone lines are formed at similar photospheric levels as weak fundamental lines and may be used alternatively. However, in the cooler stars, the strong fundamental lines provide a crucial, singular probe for the cool gas at the highest layers of the atmosphere.

Non–LTE effects in low-gravity stars complicate the interpretation of CO $\Delta v = 1$ spectra: Figure 3 compares LTE and non–LTE spectra as a function of $T_{\rm eff}$ for the $\log g = 1.5$ models. Apparently, the magnitude of non–LTE effects does not depend strongly on effective temperature for $T_{\rm eff} \leq 5000$ K. One reason for this is the weak temperature dependence of the collisional H-CO relaxation rates at a given mass column density. From hydrostatic equilibrium and the ideal gas law,

$$p = g\,m = n\,k\,T\;,$$

one finds that in (otherwise identical) stellar atmospheres with different $T_{\rm eff}$, the total density at a given m is inversely proportional to the kinetic temperature. In atmospheric layers where deviations from LTE are expected in CO, hydrogen exists largely in atomic form, therefore $n_{\rm H}$ is proportional to n and inversely proportional to T. The collisional de-excitation rate is approximately proportional to $n_{\rm H} T^{3/2}$, and therefore shows only a weak temperature dependence at a given mass column density. The magnitude of the deviation from LTE for a particular line then depends more sensitively on the precise

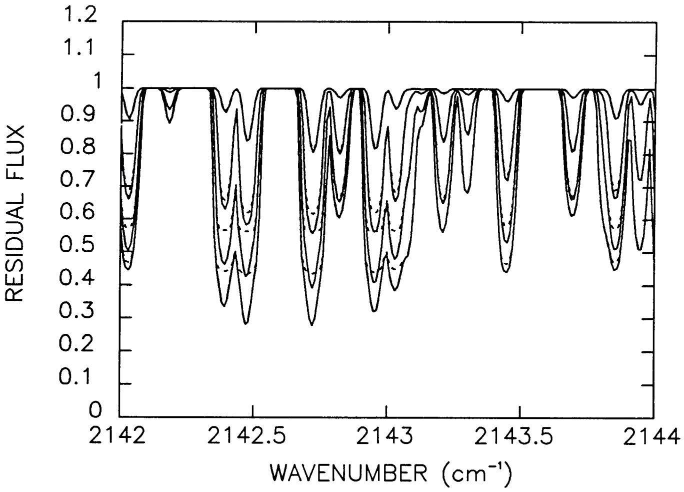

FIG. 3.—Synthetic spectra for the models with log $g = 1.5$. *Top to bottom*: $T_{\rm eff} = 6000$, 5500, 5000, and 4000 K. *Solid lines*: non–LTE spectra, dashed lines: LTE. LTE and non–LTE spectra are indistinguishable in the 6000 K model. The deviations from LTE increase with line depth.

location of line formation and the density at that altitude. Comparing the (4000, 1.5, *s*) and (5000, 1.5, *s*) models, one finds that larger departures occur in the *hotter* atmosphere in lines from higher states ($v \geq 3$): the higher vibrational states are more populated and optical depth unity for the corresponding lines occurs higher where the lower densities force smaller epsilons. In LTE models with $T_{\rm eff} \geq 5500$ K the total relative CO abundance is reduced due to dissociation and also is a stronger than linear function of the total density. A model with $T_{\rm eff} \geq 5500$ K (and lower density at a given mass column density) therefore rapidly forces $\tau = 1$ for all lines to much deeper levels of the atmosphere where LTE conditions prevail. In the (6000, 1.5, *s*) model deviations from LTE occur only at the 1% level in the strongest lines.

Summarizing, the weak temperature dependence of non–LTE effects is of importance for the use of CO lines as sensors for the stellar boundary temperature; a use for which the strongest lines are well suited. The non–LTE lines follow changes in T_b in a way very similar to the corresponding LTE lines, facilitating a differential spectrum interpretation.

c) Gravity

In stars with different surface gravities, but similar $T_{\rm eff}$, the 5 μm continuum forms essentially at the same temperature level. The different appearance of CO spectra in stars with different gravity is due to a dichotomy between the density dependences of the line and continuum opacities. The abundance of the main continuum opacity source, the negative hydrogen ion H^-, is proportional to the product of neutral hydrogen and electron densities $n_e n_{\rm H} \sim n_{\rm H}^2$. (At $T \leq 5000$ K, the electron density is proportional to the hydrogen density ($n_e \sim A_{\rm met} n_{\rm H}$) owing to the first ionizations of the abundant neutral metals at temperatures below those required to significantly ionize hydrogen itself). The CO density is a weaker function of $n_{\rm H}$, since for $T \leq 4000$ K a large fraction of all carbon atoms are bound in CO and $n_{\rm CO} \approx n_{\rm C} = A_c n_{\rm H} (n_{\rm C} < n_{\rm O})$. As a consequence, increasing g shifts the CO optical depth scales inward relative to the continuum optical depth scale. The medium-strength lines become optically thick at higher temperatures as g increases and appear shallower. However, the gravity effect diminishes with increasing $T_{\rm eff} \geq 5000$ K, where CO dissociation ($n_{\rm CO} \sim n_{\rm C} n_{\rm O}$) removes the density dichotomy between the line and continuum opacities. The "hottest" stars with $T_{\rm eff} \approx 6000$ K, where CO is largely dissociated throughout the photosphere, even produce a slight reversal of the gravity effect, although insignificant from an observational perspective. The cores of the strongest lines form in the flat part of the $T(m)$ profile and reflect the stellar boundary temperature T_b plus possible additional darkening due to non–LTE effects. T_b is determined largely by the amount of cooling in optically thin CO lines, which increases with decreasing gravity (Johnson 1973). Equally important, with the larger densities in the higher gravity models, the non–LTE line deepening is reduced owing to the faster collision rates. Non–LTE effects become insignificant in the 4000 K models (Fig. 4) for log $g \geq 3.0$. Surface gravity has negligible effect on the nature of the line formation in the 6000 K models, because LTE already is enforced at log $g = 1.5$ by the high densities in the deep-lying CO line-forming regions.

The use of CO lines as gravity probes can be summarized as follows. Weak CO lines are fairly sensitive to surface gravity in stars with $T_{\rm eff} \approx 4000$ K. Nevertheless, practical application of the depths of these lines as "gravity sensors" requires accurate and independently determined atomic abundances as input parameters to the RE models. In addition, the determination of the true continuum level in observed spectra is critical. Line intensity ratios might be more useful probes for stellar surface gravities. CO $\Delta v = 1$ spectra contain a sufficient number of weak and moderate-strength lines formed under LTE conditions, that respond differently to gravity. Depth ratios of suitable lines of the same isotopic species retain their gravity sensitivity, and are less subject to abundance determination errors.

Although the strongest lines can be affected significantly by gravity-dependent atmospheric cooling and non–LTE effects, they cannot be used to measure gravity if the temperature in the line-forming region is not predicted reliably from theoretical models or other spectral diagnostics, or if uncertainties in the magnitude of the non–LTE effects are large.

d) Abundances

The *metal* abundance of a late-type star effects the CO $\Delta v = 1$ bands directly through the effect on CO concentration

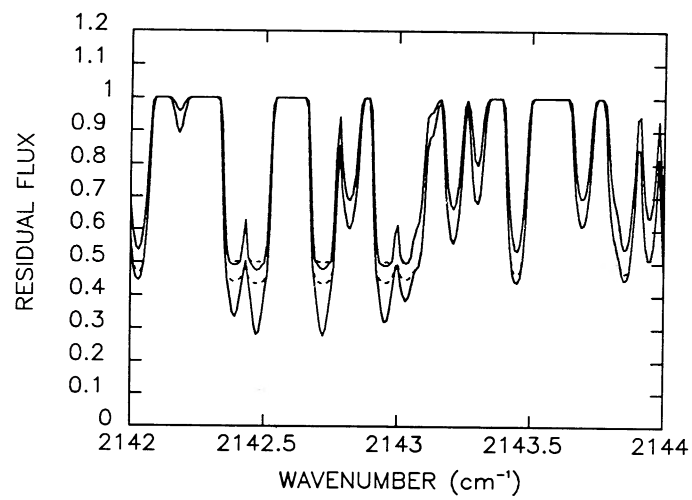

FIG. 4.—Synthetic spectra for the $T_{\rm eff} = 4000$ K models with different gravity. For clarity, only the log $g = 1.5$ (*lower line*) and log $g = 3$ (*upper line*) are shown. *Solid line*: non–LTE spectra. *Dashed line*: LTE spectra.

and indirectly through the influence on the temperature structure of the stellar atmosphere. The metal abundance determines the amount of atomic line blanketing and influences the electron density (which plays a critical role in setting the dominant continuous opacity: H^-) at temperatures below $\sim$6000 K where metal ionization dominates hydrogen ionization.

The *carbon* abundance A_C (or oxygen abundance, if it is smaller than A_C) determines at what density level the CO lines are formed, which in turn determines the magnitude of non–LTE line deepening. The second spectrum in Figure 5 was computed from the reference (4000, 1.5, *s*) model with a relative carbon abundance of 1.75×10^{-4}, (reduced by a factor of 2 from solar). The change in depth for the strong lines is almost entirely due to the reduced non–LTE line darkening at the higher densities of the deeper layers. Owing to the peripheral influence of A_C on the strong-line depths, it is crucial to determine the abundances using unsaturated CO lines ($\Delta v = 1$ or $\Delta v = 2$) or other spectral diagnostics. The inferred A_C then can serve as input parameter for the temperature determination in the region where the strong lines are formed, above the layers simulated in the current theoretical RE-atmosphere models.

Isotopic abundances: CO overtone lines are well established as tools to determine the isotopic ratios $^{12}C/^{13}C$, $^{16}O/^{18}O$ and $^{16}O/^{17}O$. The $\Delta v = 1$ lines offer an important addition: the intensities of the *double isotopic* lines $^{13}C^{18}O$ and $^{13}C^{17}O$ are too weak to be observed in overtone spectra, but some lines are detectable in $\Delta v = 1$ spectra of evolved giant stars and can provide additional constraints on the isotopic abundances of ^{13}C, ^{17}O and ^{18}O.

e) Chromospheres

Observations of atomic and ionic lines in visible and UV spectra have led to the construction of semi-empirical models for the upper atmospheres of a number of late-type stars (Kelch *et al.* 1978; Ayres and Linsky 1975, hereafter AL; Basri, Linsky, and Eriksson 1981). Common to these models, based mostly on the analysis of the Mg II *h* and *k* and Ca II H and K lines, is a temperature minimum at the top of the photosphere and an outward, "chromospheric" temperature rise. The nonclassical temperature inversion is thought to indicate the increasing importance of "mechanical" heating by acoustic waves or other types of disturbances, possibly "electrodynamic" in character (Cram 1987). The physical nature of the nonradiative heating is a central problem in modern stellar astronomy and solar physics and remains controversial despite several decades of empirical and theoretical work.

The chromospheric temperature rise in empirical models of red giant stars like Arcturus (αBoo, K1 III) begins below the altitude where the strong CO $\Delta v = 1$ lines form. The possibility of using CO fundamental spectra as a diagnostic for stellar chromospheres was first raised by Heasley and Milkey (1976). Carbon, Milkey, and Heasley (1976) subsequently computed CO $\Delta v = 1$ spectra for the Ayres—Linsky "Ca II" chromospheric temperature profile of Arcturus and later compared with the 4 m FTS spectrum in the 4.6 μm region obtained by Heasley *et al.* (1978). The absence of emission cores in the strongest of the observed CO $\Delta v = 1$ lines contradicted the predictions of the Ayres—Linsky model and called into question the assumption of a spatially pervasive, homogeneous temperature inversion as assumed in the Ca II work. Thus, a thorough understanding of the formation of the CO fundamental bands in chromospheric atmospheres, especially the magnitude and consequences of non–LTE effects, is crucial, in view of the dilemma posed by the apparently contradicting results of the IR and visible/UV diagnostics.

Figure 6 illustrates the CO $\Delta v = 1$ spectrum computed from the Kelch *et al.* (1978) model for αTau (K5 III). The strong lines become optically thick well above the temperature minimum and reflect the atmospheric temperature inversion with core emission reversals. The emission cores are partially negated in the non–LTE spectrum of αTau: the non–LTE line deepening is strong enough to destroy the weak inversions of the higher vibrational lines. However, the stronger cores of the lower vibrational lines form at higher altitudes where the temperature increase tends to reduce the non–LTE effects. In addition, the radiation fields in the strongest lines become thermalized above T_{min}, thereby preserving the emission cores.

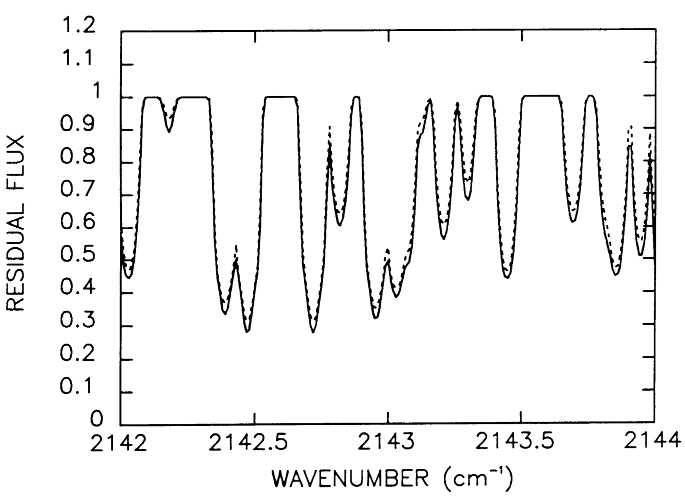

FIG. 5.—The effect of reduced carbon abundance on CO $\Delta v = 1$ spectra. *Solid line*: non–LTE spectrum of the basic (4000, 1.5, *s*) model. For the dashed spectrum, A_C was reduced by a factor of 2 relative to solar.

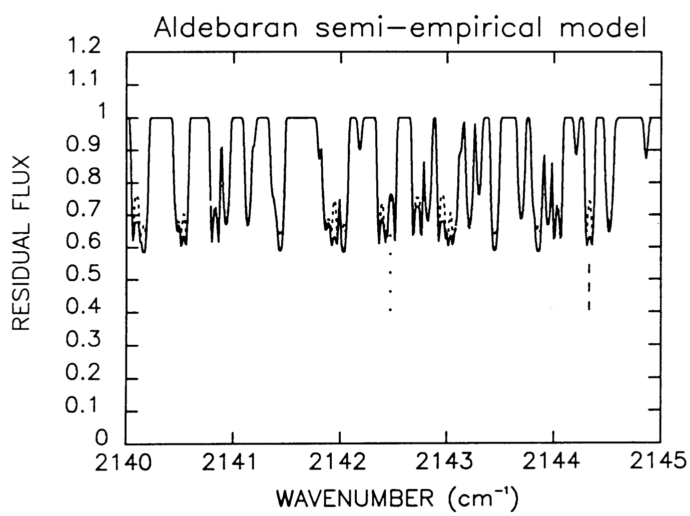

FIG. 6.—LTE and non–LTE spectra for the chromospheric model of αTau (Kelch *et al.* 1978). Core emission reversals are only partially negated by non–LTE effects (*solid curve*). The core of the strong line 2–1 R6(······) is formed high in the chromosphere under quasi–LTE conditions. The LTE-core emission reversal of 5–4 R34 (*dashed curve*), formed lower in the chromosphere, is largely destroyed by the non–LTE line deepening.

No realistic choice of CO-H collision rates eliminates the emission cores in the strong lines of the chromospheric spectrum of αTau. The situation is repeated in the chromospheric model of Arcturus (AL), where higher densities and temperatures force the CO line formation even closer to LTE (see Paper I).

f) *Effect of Uncertain Collisional Cross Sections*

i) *Magnitude*

To test the effect of uncertain collisional relaxation rates quantitatively, we computed spectra from the reference (4000, 1.5, *s*) model, varying the magnitude and *v*-dependence of the CO-H collision rates.

Figure 7 illustrates the effect of uncertain CO-H collisional cross sections. The impact of very small collisional epsilons is demonstrated by the lowest (*dashed curve*) spectrum: it was computed with relaxation rates similar to the scaling laws of Millikan and White (1963, hereafter MW), based on collisions of CO with inert perturbers like He and Ar. That result, however, does not carry much weight, since all CO-H experiments performed since MW's work agree on rates at least one order of magnitude faster. The spectra drawn in solid lines in Figure 7 were conputed with collisional cross sections increased (decreased) by a factor of 2 over the GK rates, approximately the upper (lower) limits of the experimental results. The 2 times faster rates would be similar to those derived from Wight and Leone's (1983) molecular beam experiment. The deviations from LTE become smaller for the larger collisional cross sections. The use of different collisional cross sections affects the line formation in the following way (for reduced cross sections): first the τ-scale for a particular line is shifted with respect to *m* according to the changes in the state distribution and the departure coefficients. Optical depth unity for transitions from $v = 0$ occurs at *higher* altitudes (with smaller epsilons) as b_0, the departure coefficient for the vibrational ground state, increases slightly. In addition, the reduced c_{ij}'s cause more mixing of the radiation field J_ν, thereby deepening the lines. However, 1–0 lines (especially *P*-branch transitions) that form at similar altitudes as higher vibrational

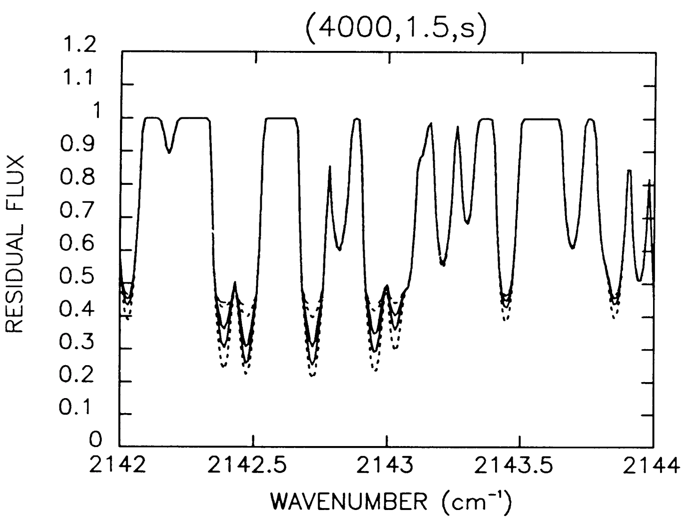

FIG. 7.—The effect of CO-H collisional cross sections on the strongest lines in CO $\Delta v = 1$ non-LTE spectra. *Solid lines*: CO-H reaction rates (GK) increased (reduced) by a factor of 2. These spectra correspond approximately to the experimental errors in the GK rates. *Lower dashed line*: Spectrum computed with the MW rates. *Upper dashed lines*: computed with RTT rates and LTE spectrum.

lines are less affected by non-LTE conditions in the first place because of their smaller A_{ij}'s. At the same time, the departure coefficients for the higher vibrational levels become smaller than unity, if the c_{ij}'s are reduced. Accordingly, the location of line formation shifts inward toward higher densities and slightly counteracts the weaker coupling to the local conditions. Interestingly, for the flat temperature profiles of our 4000 K models small deviations from LTE in the strongest CO lines occur even for collisional cross sections larger than the controversial high values proposed by von Rosenberg, Taylor, and Teare (1971). In order for deviations from LTE to be less than 1%, the collisional epsilons at $\tau = 1$ have to be in excess of 50, which is not realized in low-gravity red giant atmospheres, even with the largest plausible collision rates.

The variations in CO spectra introduced by reasonable uncertainties in the CO-H relaxation rates are less than 10% of the line intensities for the strongest absorptions in the (4000, 1.5, *s*) model, which is comparable to present observational uncertainties and other sources of error for many stars. Since the consequences of uncertain c_{ij}'s are model-dependent, a sensitivity evaluation of collisional cross sections should be performed for any interpretive non–LTE modeling of a specific star. Because of the multiplicity of CO vibration-rotation transitions in the infrared, the lines least subject to non–LTE effects can be identified and utilized.

ii) *v-Dependence*

While there is a considerable body of experimental data on the magnitude of inelastic cross sections for atom-diatom collisions, the dependence on vibrational quantum number has barely been studied owing to a variety of technical difficulties. The assumption $c_{ij} \sim A_{ij}$ has been used in previous investigations (e.g., Hinkle and Lambert 1975). This leads to *v*-independent "collisional epsilons." However, the relation most likely does not hold for inelastic CO-H collisions, where the formation of temporary chemical complexes is crucial, but rather for molecule-molecule collisions where vibrational energy transfer is dominated by other mechanisms (Bray 1968).

Nevertheless, if the collisional rates for all states are scaled according to the state's vibrational quantum number, progressively stronger coupling to local conditions occurs for the higher vibrational states. The major reduction in non–LTE effects is concentrated in the $v = 2$–4 states compared to the case of *v*-independent cross sections: the consequences are smaller for the $v > 4$ states whose lines form deep in the atmosphere, already close to LTE. Similarly, a reduction of the collisional cross sections with increasing *v*, as suggested by the experiment of Fink and Comes (1974), tends to increase non–LTE effects mainly in low-*v* lines while, again, the higher vibrational levels are less affected.

The errors introduced by uncertain de-excitation rates naturally increase with the magnitude of the non–LTE effects themselves. The largest potential errors therefore occur in the low-gravity stars with $T_{\rm eff} \leq 5000$ K. Thus, the collision-rate *v*-dependence error analysis also should be performed for every star observed with sufficiently high precision in the CO $\Delta v = 1$ bands, in order to assign realistic uncertainties to the temperature profile deduced from the highly temperature-sensitive line core intensities.

g) *Uniqueness of Derived Stellar Profiles and Boundary Temperatures*

Uncertainties in the observations (noise and errors in the continuum determination) and in the input parameters

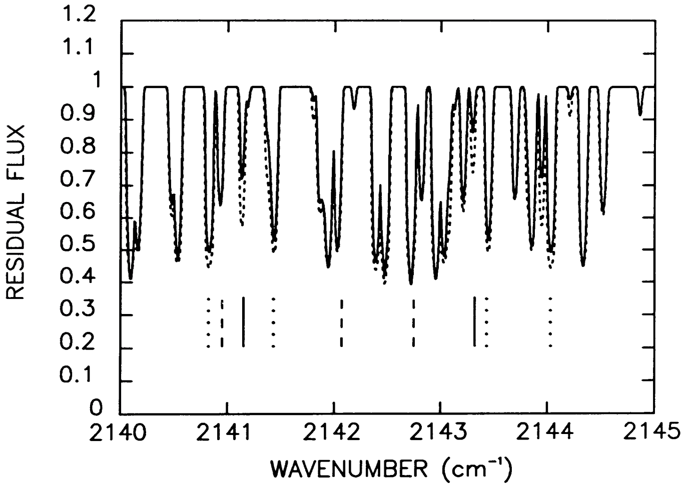

FIG. 8.—CO non–LTE spectra computed from models with different combinations of T_{eff} and g. *Solid line*: (4000, 2.25, *s*), *dashed line*: (5000, 1.5, *s*). The $^{12}C^{16}O$ lines are very similar. Discrepancies are apparent in isotopic lines. ($^{12}C^{16}O$ - - - - - -, $^{13}C^{16}O$ · · · · · ·, $^{12}C^{18}O$ ———).

(abundances, collisional cross sections, etc.) naturally extend the volume of parameter space capable of reproducing an observed spectrum. Still, the large number of lines in a measured CO $\Delta v = 1$ spectrum and the possibility of enhanced isotopic abundances in evolved stars provide many constraints for the determination of stellar parameters. For example, ostensibly similar $^{12}C^{16}O$ spectra can be produced by quite different sets of stellar parameters. The spectra in Figure 8 originate from RE model atmospheres with $T_{eff} = 4000$ K, $\log g = 2.25$ and $T_{eff} = 5000$ K, $\log g = 1.5$, respectively. The similar shapes of the photospheric temperature profiles produce the same line/continuum contrasts for the weaker lines ($v = 7 - 6$). The higher boundary temperature of the 5000 K model is compensated by the reduced non–LTE line deepening at the higher densities of the (4000, 2.25, *s*) model. The agreement is excellent except for the 2–1 R6 line which strengthens in the cooler model. The discrepancy becomes more obvious if enhanced ^{13}C and ^{18}O abundances generate an isotopic spectrum whose depth range overlaps with the $^{12}C^{16}O$ spectrum. The excitation state energies are similar in all CO molecules of different isotopic composition, as a result of the small corrections due to the reduced masses. Consequently all species respond in similar ways to temperature. However, owing to the differences in the absolute abundances, the isotopic spectra are formed at different altitudes. The optical depth scales for isotopic lines are shifted inward relative to the more abundant species. If the isotopic abundances are accurately known, e.g., from CO $\Delta v = 2$ spectra, then the $^{12}C^{16}O$, $^{13}C^{16}O$ and $^{13}C^{18}O$ bands can be considered one diagnostic tool applied to three different depth ranges.

In our observational study (Wiedemann *et al.* 1990), effective temperature, gravity and abundances are treated as input parameters, with the goal to derive the temperature structure of the outer atmospheric layers that give rise to the CO $\Delta v = 1$ spectrum. Uncertainties in the stellar effective temperature are proportionally passed on to the boundary temperature T_b. Errors for T_{eff} in well investigated stars (e.g., βGem, αTau, αBoo) are ± 200 K (Kelch *et al.* 1978) or less, if stellar diameter measurements are available, with corresponding uncertainties in T_b of $\leq \pm 100$ K. The ratio of T_b and T_{eff}, used to quantify the agreement between observed and theoretical spectra, is much less affected by the accuracy of T_{eff}.

Uncertain elemental abundances also lead to ambiguities in the derivation of T_b. A reduction of the carbon abundance by a factor of 2 in the (4000, 1.5, *s*) model is equivalent (in terms of line depths interpretation) to an increase of T_b by 120 K. However, the C and O abundances are known to within ± 0.2 dex in the brightest stars (Tsuji 1986; Lambert and Ries 1981; Smith and Lambert 1985). Thus T_b should be affected negligibly.

The most serious ambiguities in the measurement of stellar boundary temperatures arise from the uncertain magnitude (CO-H cross sections) and excitation-state dependence of the non–LTE effects. An additional contributor are errors in the surface gravity, which affects the density and thus the collision frequency. Uncertainties in the surface gravities of cool giants of ± 0.2 dex (e.g., Kelch *et al.* 1978), are equivalent to a comparable uncertainty in the hydrogen density. Errors in the CO-H collision rates affect the boundary temperature in the same way, but are ~ 3 times larger. For the (4000, 1.5, *s*) reference model with $T_b = 2400$, varying the CO-H cross sections within the experimental limits produces a ± 150 K change in the inferred T_b.

IV. CONCLUSION

Our sensitivity study demonstrates that CO fundamental spectra are in fact useful probes for the temperature structure of the outer layers of cool stellar atmospheres. Their value is limited by the uncertainties introduced by non–LTE effects, which however are reasonably small in stars with surface gravities of $\log g \approx 1.5$ and greater.

The surface gravity and other stellar parameters affect the CO line formation, but cannot easily be measured via CO $\Delta v = 1$ spectra themselves. These quantities must be determined otherwise and serve as input parameters for the CO spectrum interpretation. Fortunately, classical astronomy has provided an array of techniques for obtaining the crucial stellar parameters. Thus, the great promise of the CO spectral thermometer can be realized in practice.

We are grateful to R. Bell at the University of Maryland for providing the BEGN models in magnetic tape. G. W. acknowledges the support by the Planetary Systems Branch of the Laboratory for Extraterrestrial Physics at the Goddard Space Flight Center. T. R. A. gratefully acknowledges support from NSF (AST 88-20231) and NASA (NAG5-1215).

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