Detection of Water Vapor in the Photosphere of Arcturus

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ABSTRACT

We report detections of pure rotation lines of OH and H\textsubscript{2}O in the K1.5 III red-giant star Arcturus (α Boötis) using high-resolution, infrared spectra covering the regions 806 – 822 cm\textsuperscript{-1} (12.2 – 12.4 μm) and 884 – 923 cm\textsuperscript{-1} (10.8 – 11.3 μm). Arcturus is the hottest star yet to show water-vapor features in its disk-averaged spectrum. We argue that the water vapor lines originate from the photosphere, albeit in the outer layers. We are able to predict the observed strengths of OH and H\textsubscript{2}O lines satisfactorily after lowering the temperature structure of the very outer parts of the photosphere (\textit{log} τ\textsubscript{500} = \textit{−}3.8 and beyond) compared to a flux-constant, hydrostatic, standard MARCS model photosphere. Our new model is consistently calculated including chemical equilibrium and radiative transfer from the given temperature structure. Possible reasons for a temperature decrease in the outer-most parts of the photosphere and the assumed break-down of the assumptions made in classical model-atmosphere codes are discussed.

\textit{Subject headings:} stars: individual (α Boo) – stars: atmospheres – stars: late-type – infrared: stars

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1. INTRODUCTION

Water is one of the most abundant molecules in the atmospheres of oxygen-rich, late-type stars. It is a dominant source of opacity in the infrared and, therefore, plays an important role in determining the structure of cool photospheres. Water is prominent in the spectra of brown dwarfs, M-dwarfs and Mira variable stars. Water vapor is, however, not expected in the photospheres of giant stars hotter than late M-type [see, for example, the discussion in Tsuji (2001)]. Here, we will present evidence for water vapor in the mid-infrared, photospheric spectrum of the K1.5 III\(^3\) red giant Arcturus (α Boötes), the hottest star yet to have shown water-vapor absorption lines.

Mid-infrared, water-vapor lines have earlier been observed in sunspot spectra. Wallace et al. (1995) reported on the identification of numerous, resolved water-vapor lines in a sunspot spectrum of the N-band (760 − 1233 cm\(^{-1}\)). Polyansky et al. (1997b) were later able to assign quantum numbers to these lines, which is a very difficult task due to the great complexity of the water vapor spectrum. Wallace et al. derived an effective temperature of the observed sunspot of approximately 3300 K, which corresponds to a spectral class of M2-5. Jennings & Sada (1998) identified water-vapor lines at 811 − 819 cm\(^{-1}\) of the M-type supergiants α Orionis (Betelgeuse; M1\(^2\)) and α Scorpii (Antares; M1.5\(^2\)). These were observed at a resolution of \(R \approx 10,000\). Jennings & Sada modelled their observations with a plane-parallel, isothermal, single layer close to the location of the onset of the chromospheric temperature rise.

In order to explain several discrepancies between models and near-infrared observations of late K and M giants and supergiants, also showing water vapor, Tsuji and collaborators (see for example Tsuji et al. 1997, 1998; Tsuji 2000a,b; Yamamura et al. 1999) have introduced the idea of a stationary, warm envelope situated at a distance of a few stellar radii above the photosphere but interior to the cool, expanding circumstellar-shell. This previously undetected envelope (called the MOLsphere) is considered to contain water vapor at temperatures of 1000–2000 K (Tsuji et al. 1997), resulting in non-photospheric signatures in IR spectra of M giants. The envelope was neither theoretically predicted nor has it as yet received a theoretical explanation, but the water lines and bands seem to be a common feature of M supergiants and M giants (Tsuji et al. 1998; Matsuura et al. 1999). Numerous pieces of evidence have been presented in favor of this idea (see for example Tsuji et al. 1997, 1998; Tsuji 2000b). Here, we will, however, argue that the water-vapor lines detected in the observations of α Boo are not from a MOLsphere but of photospheric origin, a possibility anticipated by Tsuji (1988).

\(^3\)http://simbad.u-strasbg.fr/
Very little work has been done on resolved molecular lines in the mid-infrared region. Our analysis is based on spectra of Arcturus obtained with the TEXES spectrograph, a unique, high-resolution, mid-infrared spectrograph. This is the first time, to our knowledge, this wavelength region has been observed at high-resolution with high sensitivity. In Section 2 we present the observations and in Sect. 3 we identify the observed features and present our line lists which are used in the generation of synthetic spectra, a process described in Sect. 4. Section 5 we discuss our findings.

2. OBSERVATIONS

We observed Arcturus at 806.3–821.4 cm\(^{-1}\), 883.8–901.6 cm\(^{-1}\), and 903.6–922.7 cm\(^{-1}\) on 2001 February 2, 4, and 3, respectively, with the Texas Echelon-Cross-Echelle Spectrograph (TEXES; Lacy et al. 2002) mounted on the 3 meter NASA Infrared Telescope Facility (IRTF). TEXES is a ground-based prototype of EXES, a mid-infrared (350–1800 cm\(^{-1}\)) spectrograph designed for use on SOFIA (the Stratospheric Observatory For Infrared Astronomy). We observed with a resolving power of \(\tilde{\nu}/\Delta \tilde{\nu} \approx 80,000\), \(\tilde{\nu}\) being the wavenumber. A sample of the observed spectrum at 815–817 cm\(^{-1}\) is shown in Figure 1. The lines identified by comparing with the sunspot spectrum (Wallace et al. 1994) are pure rotation lines of water vapor and OH. The rotational lines of OH come in quartets. We have identified 17 water-vapor lines in the observed spectra. Several aluminum, silicon, and magnesium lines are also detected, most of which are seen in emission. These metal lines will be dealt with in a subsequent paper.

TEXES has a 0.9 meter long, aluminum echelon grating (blaze angle 84\(^{\circ}\) or R10) and a choice of an echelle or first order grating for cross-dispersion. The detector array is a 256\(^2\) pixel, Si:As IBC from the Raytheon Infrared Center for Excellence and designed for low backgrounds such as in the Space Infrared Telescope Facility (SIRTF) or high resolution spectroscopy. We used the TEXES ‘hi-lo’ spectral mode with the echelon grating cross-dispersed by the first order grating. This mode provides large spectral coverage at the cost of a short slit. It is appropriate for observing bright point sources in stable atmospheric conditions, as were present during these observations. The on-source integration times ranged from 1-2 minutes. Arcturus and Sirius, a hot star intended to be an atmospheric calibrator, were observed in the same fashion: four to six (depending on the night) 1 second integrations.

Fig. 1.— Part of the observed Arcturus spectrum at 815 – 817 cm\(^{-1}\) showing two strong OH(\(v = 0 \leftarrow 0\)) lines and several H\(_2\)O lines. Data from four orders are shown, with three inter-order gaps visible.
on the target followed by the same number of integrations on blank sky five arcseconds away. At this distance from bright stars there is an insignificant amount of scattered light. We repeated this cycle either 16 or 32 times to reach the final integration time. As part of each observation set, we also observed a telescope-temperature black-body and a sky frame for flat-fielding and wavelength calibration, as described below.

The data were reduced using the standard TEXES pipeline with flat-fielding, atmospheric correction, wavelength calibration using atmospheric lines, and optimal extraction of the spectrum. We create a flat field and first order atmospheric calibration frame by subtracting the sky frame from the black-body frame. The sky frame contains emission from telluric atmospheric lines according to the line optical depth and species temperature structure within our atmosphere. This provides a measure of the instrumental response to uniform illumination where the atmosphere is clean and gives an approximate correction for regions affected by the telluric atmosphere. We establish a frequency scale by specifying the pixel value and frequency of one atmospheric line in one order and calculating, based on our understanding of the TEXES optical components, the frequency scale for each order on the array. This process is subject to a systematic offset of as much as a few km s\(^{-1}\) if the pixel value is in error such as might happen when the only telluric lines available are fairly broad with poorly defined minima or if the only lines fall near ends of echelon orders. Normally, though, the accuracy is estimated to be on the order of ±0.5 km s\(^{-1}\), since one pixel represents roughly 0.9 km s\(^{-1}\).

After reading the data into software, we remove background emission by taking the difference of target frames and blank sky frames. After flat-fielding, we re-sample the array so that the spectral and spatial dimensions are orthogonal and run along rows and columns. We use the spatial profile of the star to construct a weighting function for optimal extraction of the stellar flux. We then have a 1D spectrum of the star.

Unfortunately, we have found that the black-body frame can result in a non-linear array response causing structure across the orders and improper atmospheric correction. We normalized each order by fitting fourth-order polynomials to the continuum and dividing. In a few orders, for example near 808 cm\(^{-1}\) and 814 cm\(^{-1}\), the normalization procedure is hampered by stellar and telluric lines. Because the signal-to-noise (S/N) in Arcturus was so high, approximately four times the S/N in the atmospheric calibrator, Sirius, we chose to make final atmospheric corrections using an atmospheric modelling program written by Erik Grossman (private communication). After a general correction, a second correction was made for just the telluric water lines since water is highly variable in Earth’s atmosphere. Since this spectral region is relatively free from telluric lines, the atmospheric correction should not significantly alter our results.
The array also seems to exhibit charge trapping after bright illuminations. The trapped charges are released during subsequent frames with a several second time constant, resulting in slightly elevated background levels. We simply ignore the first target-sky pair of each observation cycle after observing the black-body calibrator, where this effect is most prominent.

3. FEATURE IDENTIFICATION AND LINE-LISTS

Arcturus has a well determined and stable radial velocity which we exploit to check the attribution of the pure rotation OH and H$_2$O lines to the photosphere. The heliocentric velocity is $-5.2\,\text{km\,s}^{-1}$ (Evans 1979) stable to about $0.1\,\text{km\,s}^{-1}$ (Hatzes & Cochran 1993). Our measured line positions are corrected for this velocity and the contribution from the Earth’s velocity in order to obtain velocity shifts with respect to the photospheric velocity.

3.1. Vibration-Rotation OH Lines

The OH radical is an expected photospheric constituent. Vibration-rotation lines from the molecule’s ground state are securely identified in the infrared Arcturus Atlas (Hinkle et al. 1995a,b). We use a selection of the first-overtone lines near 1.6$\mu$m to establish the photospheric contribution to the pure rotation OH lines. In this section, we compare vibration-rotation and pure rotation lines with respect to velocity and line width. We later discuss the observed line strengths.

Figure 2 shows several OH lines from the Hinkle et al. Atlas. Laboratory line positions from Goldman et al. (1998) via Melen et al. (1995) are accurate to about 0.0038 cm$^{-1}$ or 0.2 km s$^{-1}$. The data in Table 1 are measured off the Arcturus Atlas. Also presented are line data from the Goldman et al. (1998) line-list. Oscillator strengths given in the Table as log $gf$-values are taken from Goldman et al. (1998) and are considered accurate to about 10%.

Fig. 2.— Part of the analyzed Arcturus spectrum around 1.6$\mu$m. The OH($\nu' - \nu'' = 2 - 0$) lines are fitted well with a standard MARCS photospheric model. The data are plotted with crosses and the model is shown with a full line. Several metal lines are present. No attempt has, however, been made to fit the abundances or uncertain $gf$-values of individual metal lines, nor has an attempt been made to make a complete line list for the region. The focus has been on the vibration-rotation OH lines. The regularly spaced narrow spikes in the spectrum are residuals from telluric water vapor lines after division of a telluric spectrum.
Observed line positions scatter about the adopted photospheric velocity: the mean velocity shift is \( \langle \Delta \tilde{\nu}_{\text{OH}(6400)} \rangle = 0.1 \pm 0.2 \text{ km s}^{-1} \). The mean measured width (FWHM) is 8.8 \( \pm \) 0.3 km s\(^{-1}\) (see Table 1). The Atlas resolution corresponds to a line width of about 1.9 km s\(^{-1}\) implying that the true width of the OH lines is approximately \( \sqrt{8.8^2 - 1.9^2} = 8.6 \pm 0.4 \text{ km s}^{-1} \).

### 3.2. Pure Rotation OH Lines

Observed, mid-infrared, pure rotation lines are summarized in Tables 5 and 4. Laboratory line positions are accurate to about 0.0004 cm\(^{-1}\) or 0.15 km s\(^{-1}\) (Goldman et al. 1998). We use line data from the Goldman et al. (1998) line list and the assignments in the Table are from the mid-infrared Atlas of the sunspot spectrum (Wallace et al. 1994). The continuum around 919.7 cm\(^{-1}\) is not well defined due to spurious features due to telluric absorption there, severely affecting the measurements. The observed lines are at the photospheric velocity. For the three observational sets the values are: \( \langle \Delta \nu_{\text{OH}(810)} \rangle = -0.4 \pm 0.2 \pm 0.5 \text{ km s}^{-1} \), \( \langle \Delta \nu_{\text{OH}(890)} \rangle = 1.4 \pm 0.1 \pm 1.5 \text{ km s}^{-1} \), and \( \langle \Delta \nu_{\text{OH}(910)} \rangle = -0.7 \pm 0.2 \pm 0.5 \text{ km s}^{-1} \), see Table 5 and 4. After the standard deviation of the mean, the estimated systematic uncertainties are given. The latter is generally estimated to \( \pm 0.5 \text{ km s}^{-1} \), but the OH (and H\(_2\)O) lines from the February 4 spectra are shifted by about 1.5 km s\(^{-1}\) relative to the photospheric velocity, a shift not seen in the February 2 and 3 observations. We, therefore, suppose that the anomalous shift arises from the wavelength calibration of the February 4 spectra.

The measured line widths of the measured 1 – 1, 2 – 2, and 3 – 3 OH lines give a mean FWHM of 8.8 \( \pm \) 0.3 km s\(^{-1}\). The instrumental profile corresponds to a FWHM of about 3.7 km s\(^{-1}\). Correcting for this, the intrinsic width of these OH lines is about 7.9 \pm 0.4 km s\(^{-1}\), which is in fair agreement with the width of the vibration-rotation OH lines.

The photosphere is certainly home to the OH molecules giving the vibration-rotation lines. By velocity and FWHM similarities, the suspicion is strong that the pure rotation lines are also of photospheric origin. Below (Sec. 5) we further the argument for this origin by comparing synthetic and observed spectra.

### 3.3. H\(_2\)O Lines

A call for adequate representation of the line opacity from H\(_2\)O molecules needed in construction of model photospheres of cool stars has been answered by the construction of line lists using techniques of theoretical molecular spectroscopy. For example, the scan list (Jørgensen et al. 2001) contains 100 million lines with predicted wavelengths and line
strengths. Partridge & Schwenke (1997) combine predictions with laboratory measurements. Available line lists are discussed by Jørgensen et al. (2001) and Bernath (2002). Present line lists are likely satisfactory for an opacity calculation and probably for comparing synthetic and observed low resolution spectra (see, for example, Jones et al. 2001 and Ryde & Eriksson 2002), but our need for precise line positions cannot be met by theoretical calculations. Partridge & Schwenke’s calculations match laboratory measurements of line positions to about 0.05 cm$^{-1}$ or about 20 km s$^{-1}$ for the lines of interest to us.

Therefore, we take line positions from laboratory measurements of strong H$_2$O lines (Polyansky et al. 1996, 1997a,b). These measurements made at a resolution of $\Delta \tilde{\nu} \approx 0.01$ cm$^{-1}$, provide wavenumbers, excitation energies of the lower state of the transition, and quantum state assignments (with the rotational quantum numbers $J$, $K_a$, and $K_c$) of the ground vibrational state, $(v_1v_2v_3) = (000)$, and the first excited bending vibrational state, $(v_1v_2v_3) = (010)$. These are states that give rise to relevant transitions for our study. The uncertainty in the line positions is less than 0.002 cm$^{-1}$ (P. Bernath 2002, private communication). By using the excitation energies of the measured lines, we are able to identify the corresponding lines in the line list by Partridge & Schwenke (1997), which provides us with accurate transition probabilities ($gf$ values). The excitation energies (to be used in the calculation of the level populations) in Polyansky et al. (1996, 1997a) and Partridge & Schwenke (1997) agree excellently with the experimentally measured energy levels of Tennyson et al. (2001). We use the partition function for water from Partridge & Schwenke (1997) in our calculations of the synthetic spectra. Our new list of water-vapor lines is presented in Tables 2 and 3. The line positions and assignments are given as in Polyansky et al. (1996, 1997a). The $gf$ values and the excitation potentials are taken from Partridge & Schwenke (1997).

In order to test the wavelength accuracy of our new line list, we compared with the sunspot spectrum (Wallace et al. 1994) finding a good agreement within the uncertainties of the line lists. We are therefore confident that the wavelengths of the few water-vapor lines, used in the compilation of our new line list, are accurate.

Single, unblended H$_2$O lines are expected to be the rule when H$_2$O contributes weakly, as in the Arcturus spectrum. But there are certainly blends of water-vapor lines not accounted for in our line list. Indeed, in the Partridge & Schwenke (1997) line list, we detected a number of lines sufficiently strong to affect the synthetic spectrum within one or a few resolution elements of a measured line (assigned by Polyansky and collaborators). We, therefore, also included these lines in our list with the (uncertain) wavelength shifts found in the Partridge

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$K_a$ is the approximate projection of the total angular momentum, $J$, along the rotational axis with the smallest momentum of inertia and $K_c$ is the corresponding projection along the rotational axis with the largest momentum of inertia.
In Tables 2 and 3 these extra lines are given with only 6 digits, whereas the Polyansky et al. (1996, 1997a) lines are given with 8 digits (as is given in these references). Some missing lines and blends may also affect our synthetic spectrum. We also note that the Partridge & Schwenke line list shows artificial splittings of a large number of degenerate, rotational states, which could make assignments difficult (see the discussions in Polyansky et al. 1997b; Jones et al. 2001; Ryde & Eriksson 2002).

In Tables 2 and 3 measurements of stellar water-vapor lines are shown. The mean velocity shifts of the observed lines relative to the stellar velocity are negligible: \( \langle \Delta v_{(810)} \rangle = 0.1 \pm 0.2 \pm 0.5 \, \text{km s}^{-1}, \langle \Delta v_{(890)} \rangle = 1.6 \pm 0.2 \pm 1.5 \, \text{km s}^{-1}, \) and \( \langle \Delta v_{(910)} \rangle = -0.1 \pm 1.1 \pm 0.5 \, \text{km s}^{-1}. \) In comparing the velocity shifts of the OH and water lines in the 800–822 cm\(^{-1}\) region (which has most measured values), we note that the systematic, instrumental shifts will be the same for both species. Thus, there might be a small red-shift of the \( \text{H}_2\text{O} \) lines relative to the OH lines of \( 0.5 \pm 0.3 \, \text{km s}^{-1}. \) A velocity shift of this order is indeed expected between lines formed at different depths in the photosphere in a star such as Arcturus, see for example Allende Prieto et al. (2002). The FWHM of the water-vapor lines is measured to be \( \langle \text{FWHM} \rangle = 8.2 \pm 0.3 \, \text{km s}^{-1} \). Correcting for the intrinsic line width, we find \( \langle \text{FWHM} \rangle = 7.3 \pm 0.4 \, \text{km s}^{-1}, \) which is slightly lower than the line widths found for the OH lines. Thus, the water-vapor lines, by their line width and velocity, appear to be formed in the photosphere.

## 4. MODEL PHOTOSPERHERES AND THE GENERATION OF SYNTHETIC SPECTRA

For the purpose of analyzing our observations, we have generated synthetic spectra based on model photospheres calculated with the latest version of the MARCS code. This version of the MARCS code is the final major update of the code and its input data in the suite of MARCS model-photosphere programs first developed by Gustafsson et al. (1975) and further improved in several steps, e.g. by Plez et al. (1992), Jørgensen et al. (1992), and Edvardsson et al. (1993).

The MARCS hydrostatic, spherical model photospheres are computed on the assumptions of Local Thermodynamic Equilibrium (LTE) including chemical equilibrium, homogeneity and the conservation of the total flux (radiative plus convective; the convective flux being computed using the mixing length formulation). The radiative field used in the model generation, is calculated with absorption from atoms and molecules by opacity sampling at approximately 84,000 wavelength points over the wavelength range 2300 Å–20 \( \mu \text{m}. \)

Data on the absorption by atomic species are collected from the VALD database (Piskunov...
et al. 1995) and Kurucz (1995, private communication). The opacity of CO, CN, CH, OH, NH, TiO, VO, ZrO, H₂O, FeH, CaH, C₂, MgH, SiH, and SiO are included and up-to-date dissociation energies and partition functions are used. The continuous absorption as well as the new models will be fully described in a series of forthcoming papers in A&A (Gustafsson et al., Jørgensen et al., and Plez et al., all in preparation).

The model photosphere is described, for every depth point through the photosphere, by the radius \( R \), the standard optical depth calculated at 500 nm \( \tau_{500} \), temperature \( T \), electron pressure \( P_e = N_e kT \), gas pressure \( P_g = N kT \), density \( \rho \), and standard opacity at 500 nm. Normally, the models are calculated with 54 depth points from \( \log \tau_{\text{Ross}} = 2.0 \) out to \( \log \tau_{500} = -4.8 \). The physical height above the \( \log \tau_{500} = 0 \) layer of this outermost point is \( 6.2 \times 10^{10} \) cm or 3% of the stellar radius. We will use the \( \log \tau_{500} \) scale as a depth scale in the following discussion.

Using the model photosphere we calculate synthetic spectra by solving the radiative transfer in a spherical geometry. We calculate the radiative transfer for points in the spectrum separated by \( \Delta \tilde{\nu} \sim 1 \text{ km s}^{-1} \) (corresponding to a resolution of \( \tilde{\nu} / \Delta \tilde{\nu} \sim 330000 \)) even though the final resolution is lower.

Arcturus is a well studied star. The effective temperature derived by Griffin & Lynas-Gray (1999) is, for example, \( T_{\text{eff}} = 4290 \pm 30 \) K. Peterson et al. (1993) deduce its stellar parameters by synthesizing the optical spectrum using extensive line lists, and find \( T_{\text{eff}} = 4300 \pm 30 \) K, \( \log g = 1.5 \pm 0.15 \) (cgs), \( \text{[Fe/H]} = -0.5 \pm 0.1 \), and \( \xi_t = 1.7 \pm 0.3 \text{ km s}^{-1} \). Decin et al. (1997) derive the stellar parameters from studying the entire Infrared Space Observatory (ISO) spectrum (2.4 - 12 \( \mu \)m) of Arcturus. They used the same MARCS code and the same input data as we are using. Their parameters for Arcturus are \( T_{\text{eff}} = 4300 \) K, \( \log g = 1.75 \) (cgs), \( \xi_t = 1.7 \text{ km s}^{-1} \), \( M = 1 \text{ M}_\odot \), and the specific abundances \( \epsilon(C) = 7.90 \), \( \epsilon(N) = 7.55 \), and \( \epsilon(O) = 8.67 \) on the usual logarithmic scale of 12. The surface gravity of Decin et al. (1997) seems to be somewhat high in comparison with other literature values. We will, therefore, calculate our standard model with \( T_{\text{eff}} = 4300 \) K, \( \log g = 1.5 \) (cgs), \( \text{[Fe/H]} = -0.5 \), and \( \xi_t = 1.7 \text{ km s}^{-1} \), and use the abundances of carbon, nitrogen, and oxygen given by Decin et al. (1997).

We find that the temperature structure differs between a model atmosphere calculated in plane-parallel geometry and a model in spherical geometry for \( \tau_{500} \lesssim -1 \), with a maximum difference of 65 K at \( \tau_{500} \sim -4 \). To minimize the uncertainties we therefore choose to calculate our models in spherical geometry.

In order to test the stellar model we start by synthesizing Arcturus’ spectrum at
6400 cm$^{-1}$ and confront it with the high-resolution observations presented in the infrared Arcturus Atlas (Hinkle et al. 1995a,b), see Figure 2. The synthesized region, 6350–6430 cm$^{-1}$, is chosen since it contains several first-overtone, vibration-rotation OH lines ($v' - v'' = 2 - 0$ and $3 - 1$). The synthetic OH lines are narrower than their real counterparts. To match the observed widths, we introduce the customary artifice of a macroturbulent velocity. We suppose these velocities follow a Gaussian distribution. The adopted macroturbulence parameter is \( 5.7 \pm 0.5 \) km s$^{-1}$. Figure 2 shows that OH lines are fitted well with our model, indicating the relevance of the model photosphere and the stellar parameters used in modelling it. No attempt has been made to fit the metal lines, nor has an attempt been made to make a complete line list for the region. The focus has been to show that the vibration-rotation OH lines are ascribed to the star’s photosphere. This demonstration is a firm basis from which to begin interpretation of the pure rotation OH and H$_2$O lines.

Confident of the stellar parameters used in the generation of the model photosphere, we now confront the mid-infrared, high-resolution TEXES spectra with a synthetic spectrum of the 806–923 cm$^{-1}$ region, containing pure rotation OH lines and H$_2$O lines. Observed and model spectra are shown in Figures 3, 4, 5, and 6. The dashed line shows the synthetic spectra calculated with our model-photosphere. The wavenumber scale is expressed in the stellar rest frame. The synthetic, near-infrared spectrum of Arcturus was convolved with Gaussians, representing macroturbulence and the instrumental profile of 6 km s$^{-1}$. For the mid-infrared spectra, a macroturbulence parameter of \( 4.7 \pm 0.5 \) km s$^{-1}$ fits the OH lines well. To within the uncertainties, these estimates from different spectral regions and spectra obtained at different times are identical.

Given that the model and adopted abundances give an excellent fit to the 1.6 \( \mu \)m vibration-rotation OH lines, it is of interest to see if the same model-abundance combination fits the pure rotation OH lines. The answer (Figures 3–5) is that the OH(1–1), OH(2–2), and OH(3–3) lines in the synthetic spectra are a very good fit to the observed lines. The quality of the fit is poorer for the OH(0–0) lines in that the predicted lines are weaker than observed.

In comparison to the mild failure to predict the 0–0 OH lines, the failure to account for the observed H$_2$O lines is dramatic (Figure 6). It is impossible to find a MARCS model that would predict the line strengths of all H$_2$O and OH lines by only changing the effective
Table 1: Observational data of OH, vibration-rotational lines at 6350 – 6430 cm$^{-1}$.

| $\tilde{\nu}_{\text{lab}}$ | $\Delta \tilde{\nu}$ | Equivalent width | FWHM | $E'_{\text{exc}}$ | $\log gf$ | $v' - v''$ | Lower level |
|--------------------------|------------------|------------------|-------|-----------------|----------|-------------|-------------|
| [cm$^{-1}$]              | [km s$^{-1}$]    | [10$^{-3}$ cm$^{-1}$] | [km s$^{-1}$] | [eV]             |          |             |             |
| 6355.363                 | 0.05             | 55.0             | 8.0   | 0.354           | -5.24    | 2-0         | $P_{1f}12.5$ |
| 6356.868                 | 1.2              | 72.3             | 10.7  | 0.353           | -5.24    | 2-0         | $P_{1e}12.5$ |
| 6359.707                 | -0.15            | 45.4             | 7.6   | 0.358           | -5.27    | 2-0         | $P_{2e}11.5$ |
| 6360.749                 | -1.2             | 63.7             | 9.4   | 0.357           | -5.27    | 2-0         | $P_{2f}11.5$ |
| 6386.612                 | -0.32            | 46.8             | 10.4  | 0.534           | -5.17    | 3-1         | $P_{1f}6.5$  |
| 6387.258                 | -0.11            | 40.4             | 7.8   | 0.534           | -5.17    | 3-1         | $P_{1e}6.5$  |
| 6397.266                 | 0.46             | 47.1             | 9.3   | 0.541           | -5.24    | 3-1         | $P_{2e}5.5$  |
| 6397.555                 | 0.49             | 42.1             | 8.1   | 0.541           | -5.24    | 3-1         | $P_{2f}5.5$  |
| 6419.992                 | 0.70             | 57.7             | 8.9   | 0.300           | -5.29    | 2-0         | $P_{1f}11.5$ |
| 6421.354                 | 0.13             | 51.9             | 8.1   | 0.299           | -5.29    | 2-0         | $P_{1e}11.5$ |
| 6424.877                 | 0.00             | 53.7             | 8.0   | 0.304           | -5.33    | 2-0         | $P_{2e}10.5$ |

Fig. 4.— Pure rotation, OH($v = 1 - 1$) lines. See Figure 3 for an explanation for the different curves. The line at 918.8 cm$^{-1}$ contains a water-vapor blend.

Fig. 5.— Pure rotation, OH($v = 2 - 2$) lines. See Figure 3 for an explanation for the different curves.

Fig. 6.— Pure rotation, water-vapor lines. The observed spectrum is plotted with crosses. The dashed line shows the synthetic spectrum calculated based on our original model photosphere. The full line shows the spectrum based on the photosphere with the new temperature structure.
Table 2: Observational data and the line list of the water-vapor lines for the $806 - 822$ cm$^{-1}$ region from 2001 February 2.

| $\nu_{\text{lab}}$ [cm$^{-1}$] | $\Delta \nu^a$ | equivalent width$^a$ [cm$^{-1}$] | FWHM$^a$ [km s$^{-1}$] | $E''_{\text{exc}}$ [eV] | log $gf$ | $J'' K''_a K''_c J' K'_a K'_c$ | $v_1 v_2 v_3$ |
|---------------------------|----------------|-------------------------------|-------------------|-----------------|-------|-------------------------------|-----------------|
| 813.75067                | 0.18:          | 0.79:                         | 5.7:              | 0.833           | -1.90 | 23 8 15 22 7 16               | (000)           |
| 815.30059                | 0.54           | 1.3                           | 7.1               | 0.498           | -2.51 | 18 7 12 17 4 13               | (000)           |
| 815.897$^b$              | -0.74          | 0.85                          | 7.8               | 1.396           | -1.48 | 21 21 0 20 20 1               | (010)           |
| 815.900$^b$              | -0.74          | 0.85                          | 7.8               | 1.396           | -1.48 | 21 21 0 20 20 1               | (010)           |
| 816.45026                | 0.25:          | 0.26:                         | 7.2:              | 0.398           | -3.21 | 17 5 13 16 2 14               | (000)           |
| 816.68703                | 0.34           | 1.8                           | 9.3               | 1.014           | -1.35 | 24 12 13 23 11 12             | (000)           |
| 817.138                  |                |                               |                   | 1.206           | -1.66 |                              |                 |
| 817.15695                | 0.72           | 1.6                           | 9.1               | 1.206           | -1.18 | 21 16 5 20 15 6               | (010)           |
| 817.20881                | -0.69:         | 1.1:                          | 10.5:             | 1.014           | -1.83 | 24 12 12 23 11 13             | (000)           |
| 817.209                  |                |                               |                   | 1.460           | -1.55 |                              |                 |
| 818.4238$^c$             |                |                               |                   | 1.029           | -1.66 | 22 16 6 21 15 7               | (000)           |
| 818.4247$^c$             | 0.022          | 2.6                           | 8.0               | 1.029           | -1.19 | 22 16 7 21 15 6               | (000)           |
| 819.93233                | 0.089          | 0.78                          | 6.6               | 1.050           | -1.42 | 25 11 14 24 10 15             | (000)           |

$^a$A colon (:) marks measured values with large uncertainties.

$^b$Uncertain assignment of the quantum numbers for the states of the transition.

$^c$Assignments from Tsuji (2000)
Table 3: Observational data and the line list of the water-vapor lines for the 884 – 925 cm\(^{-1}\) region from 2001 February 3 and 4.

| \(\tilde{\nu}_{\text{lab}}\) [cm\(^{-1}\)] | \(\Delta\tilde{\nu}\) [km s\(^{-1}\)] | Equivalent width\(^a\) [10\(^{-3}\) cm\(^{-1}\)] | FWHM\(^a\) [km s\(^{-1}\)] | \(E''_{\text{exc}}\) [eV] | \(J'K'_{a}K'_{c}J''K''_{a}K''_{c}\) | \(v_{1}v_{2}v_{3}\) |
|-----------------|-----------------|-----------------|-----------------|-----------------|-----------------|-----------------|
| 886.042         | 1.61            | 1.0             | 8.4             | 1.265           | -1.60           |                  |
| 886.0432        | 1.34            | 1.1             | 8.4             | 0.602           | -2.40           |                  |
| 894.63740       | 1.96            | 0.94            | 7.9             | 0.626           | -2.47           |                  |
| 894.647         | -2.06           | 0.97:           | 8.3:            | 0.804           | -2.16           |                  |
| 904.62103       | 1.505           | -1.11           |                 |                 |                 |                  |
| 904.67827       | :               | :               | :               | 0.571           | -2.98           |                  |
| 910.71027       | 1.63:           | 1.1:            | 8.8:            | 0.408           | -2.99           |                  |
| 911.23428       | 0.040           | 0.78            | 7.3             | 0.489           | -2.71           |                  |
| 914.60786       | :               | :               | :               | 0.489           | -3.18           |                  |

\(^a\)A colon (:) marks measured values with large uncertainties.
Table 4: Observational data of pure rotational, OH lines at 884–925 cm$^{-1}$ from 2001 February 3 and 4.

| $\tilde{\nu}_{lab}$ [cm$^{-1}$] | $\Delta\tilde{\nu}^a$ [km s$^{-1}$] | Equivalent width$^a$ [10$^{-3}$ cm$^{-1}$] | FWHM$^a$ [km s$^{-1}$] | $E''_{exc}$ [eV] | log $gf$ | $v' - v''$ | Lower level |
|-------------------------------|-----------------|-----------------------------|----------------|----------------|---------|--------|----------|
| 883.9131                      | 1.1             | 9.5                         | 10.3           | 1.614          | -1.50   | 0-0    | R$_{2e}$26.5 |
| 884.6252                      | 1.7             | 4.3                         | 8.8            | 2.200          | -1.45   | 1-1    | R$_{1e}$29.5 |
| 885.2840                      | 1.7             | 3.6                         | 8.5            | 2.205          | -1.46   | 1-1    | R$_{2e}$28.5 |
| 885.6448                      | 1.1             | 4.8                         | 9.9            | 2.203          | -1.45   | 1-1    | R$_{1f}$29.5 |
| 891.4516                      | 2.0:            | 1.3:                        | :              | 2.872          | -1.43   | 2-2    | R$_{2f}$31.5 |
| 892.1655                      | 1.0:            | 0.98:                       | :              | 2.874          | -1.43   | 2-2    | R$_{2e}$31.5 |
| 892.4433                      | 1.4:            | 1.3:                        | 7.8:           | 2.873          | -1.41   | 2-2    | R$_{1f}$32.5 |
| 903.7739                      | -1.3            | 31.6                        | 10.5           | 1.721          | -1.47   | 0-0    | R$_{2f}$27.5 |
| 904.0414                      | -0.16           | 31.9                        | 10.6           | 1.718          | -1.45   | 0-0    | R$_{1e}$28.5 |
| 904.8001                      | 0.24            | 30.3                        | 10.0           | 1.723          | -1.47   | 0-0    | R$_{2e}$27.5 |
| 904.8011 blended with OH(0-0) |                |                             |                | 2.982          | -1.41   | 2-2    | R$_{2e}$32.5 |
| 905.0040                      | -0.42:          | 1.4:                        | :              | 2.980          | -1.39   | 2-2    | R$_{1f}$33.5 |
| 905.1867                      | -0.97           | 30.8                        | 10.2           | 1.722          | -1.45   | 0-0    | R$_{1f}$28.5 |
| 905.4647                      | -2.0:           | 0.69:                       | :              | 2.985          | -1.41   | 2-2    | R$_{2e}$32.5 |
| 905.7167                      | -0.64:          | 1.9:                        | :              | 2.983          | -1.39   | 2-2    | R$_{1f}$33.5 |
| 917.0493                      | -2.2:           | 1.0:                        | :              | 3.096          | -1.38   | 2-2    | R$_{2e}$33.5 |
| 917.2380                      | 0.53:           | 0.96:                       | :              | 3.097          | -1.39   | 2-2    | R$_{1e}$34.5 |
| 917.6575                      | -1.6:           | 0.91:                       | :              | 3.092          | -1.38   | 2-2    | R$_{2e}$33.5 |
| 917.8851                      | 0.81:           | 1.4:                        | :              | 3.095          | -1.39   | 2-2    | R$_{1f}$34.5 |
| 918.8106                      | -1.0:           | 3.2                         | 8.0:           | 2.424          | -1.42   | 1-1    | R$_{2f}$30.5 |
| 919.0291                      | -1.2            | 3.1                         | 8.1            | 2.421          | -1.40   | 1-1    | R$_{1e}$31.5 |
| 919.6607                      | -0.76:          | 4.4                         | 10.7           | 2.426          | -1.42   | 1-1    | R$_{2e}$30.5 |
| 919.9632                      | 0.046           | 3.3                         | 8.8            | 2.425          | -1.40   | 1-1    | R$_{1f}$31.5 |

$^a$A colon (:) marks measured values with large uncertainties.
Table 5: Observational data of pure rotational, OH lines at 806–822 cm$^{-1}$ from 2001 February 2.

| $\tilde{\nu}_{\text{lab}}$ | $\Delta\tilde{\nu}^a$ | Equivalent width$^a$ | FWHM$^a$ | $E''_{\text{exc}}$ | log $gf$ | $v' - v''$ | Lower level |
|-----------------------------|------------------------|----------------------|-----------|-------------------|--------|-------------|-------------|
| [cm$^{-1}$]                 | [km s$^{-1}$]          | [10$^{-3}$ cm$^{-1}$]| [km s$^{-1}$] | [eV]             |        |             |             |
| 808.9456                   | 0.03:                  | 2.5:                 | 8.1:      | 2.349            | -1.54  | 2-2         | R$_{2f}26.5$|
| 809.2817                   | -0.75                  | 2.7                  | 8.3       | 2.346            | -1.52  | 2-2         | R$_{1e}27.5$|
| 809.8358                   | -0.07                  | 2.8                  | 9.1       | 2.351            | -1.54  | 2-2         | R$_{2e}26.5$|
| 810.2738                   | -0.45:                 | 2.6:                 | 8.0:      | 2.349            | -1.52  | 2-2         | R$_{1f}27.5$|
| 814.3245                   | -0.50                  | 11.5                 | 11.1      | 1.300            | -1.59  | 0-0         | R$_{2f}23.5$|
| 814.7280                   | -1.06:                 | 12.1                 | 11.7      | 1.297            | -1.57  | 0-0         | R$_{1e}24.5$|
| 815.4032                   | -0.79:                 | 10.4                 | 10.7      | 1.302            | -1.58  | 0-0         | R$_{2e}23.5$|
| 815.9535                   | -0.92                  | 11.7                 | 11.4      | 1.300            | -1.57  | 0-0         | R$_{1f}24.5$|
| 820.4937                   | 0.68:                  | 0.72:                | 7.9:      | 2.981            | -1.50  | 3-3         | R$_{2f}29.5$|
| 821.1968                   | 0.25:                  | 0.57:                | 7.5:      | 2.983            | -1.50  | 3-3         | R$_{2e}29.5$|

$^a$A colon (:) marks measured values with large uncertainties.
temperature and surface gravity. Some water-vapor lines can be fitted by a 4100 K model whereas others can only be synthesized with a 3900 K model. The OH($v = 0 - 0$) lines need even lower effective temperatures: approximately 3000 K. Higher surface gravities tend to strengthen the lines. Such a failure must hold novel information about Arcturus’ atmosphere. Given that the H$_2$O lines are at the photospheric velocity and have the width of the photospheric OH vibration-rotation and pure rotation lines, we argue that the H$_2$O lines are also photospheric lines. It should also be noted that circumstellar emission or infrared excess of thermal radiation from dust is not seen from Arcturus, a conclusion demonstrated by the ISO fits of the star’s 2.4 – 12 μm spectrum (Decin et al. 1997). Thus, the failure is taken to be a signal that the model photosphere and/or the synthetic spectrum is an inadequate representation of the real photosphere. Were the H$_2$O lines formed in a detached layer such as a MOLsphere it seems likely that their velocity, line width, and degree of excitation would not match so closely the photospheric values.

5. DISCUSSION

The presence of a detectable column density of H$_2$O in Arcturus’ photosphere is at odds with our predictions which combine an appropriate MARCS model with a spectrum synthesis code. One or more aspects of the combination must be in need of revision. In this section, we comment on some possible revisions.

5.1. A Cooler Upper Photosphere?

Perhaps, the simplest revision providing stronger predicted H$_2$O lines is to drop the temperatures in the uppermost, uncertain layers of the model photosphere. MARCS models are normally begun at log $\tau_{500} = -4.8$ and extend into the star. To assure ourselves that an outward extension would not affect the synthetic spectra, we recomputed the MARCS model

Fig. 7.— The temperature and gas-pressure structures of our models. The full line shows the original MARCS model. The dotted line shows the same model but from a new calculation extending it further out. The dashed line shows our model that fit our observations, with a modified T-structure at log $\tau_{500} < -3.8$ and beyond. The electron and gas pressures and the density are calculated consistently from this temperature structure. The apparent difference in the gas-pressure structure between the original model (full line) and its extension (dotted line) is most likely a numerical boundary effect in the original model.
with the first depth point at \( \log \tau_{500} = -7.0 \), corresponding to \( 8.8 \times 10^{10} \) cm, or 4% of the stellar radius, above the \( \log \tau_{500} = 0 \) layer. The OH and H\(_2\)O lines in the synthetic spectrum are almost unchanged; the predicted H\(_2\)O lines remain far weaker than observed. A helpful reference mark in discussions of model structure is the location of optical depth unity in the mid-infrared continuum: \( \tau_{12\mu m} = 1 \) occurs at \( \log \tau_{500} = -0.5 \).

After one or two tests, it became clear that a minor revision of temperatures in the extreme boundary layers suffices to impose strong H\(_2\)O lines on the synthetic spectrum. By cooling the temperature structure, water vapor starts to form in the outer layers. We find that the strengths of the water lines are very sensitive to the temperature structure of the very outer photosphere. In Figure 7, we show an alternative choice for the temperature in this boundary layer with temperatures cooler than the MARCS model for \( \log \tau_{500} < -3.8 \); the model now violates the condition of flux constancy imposed on MARCS models. Over most of the region, the temperatures are a mere 300 K cooler than the MARCS model. Electron and gas pressures were recalculated assuming hydrostatic equilibrium. The density and standard opacity are also consistently recalculated from this new temperature structure, as are the ionization balance, molecular equilibria, and opacities. New synthetic spectra were calculated assuming, as before, LTE for the molecular equilibrium and the line formation.

The new spectra (solid lines in Figures 3 – 6) provide a pleasing simulation of the observed OH and H\(_2\)O lines. The OH vibration-rotation lines at 6400 cm\(^{-1}\) and the OH pure rotation \( 3 - 3, 2 - 2, \) and \( 1 - 1 \) lines are unaffected by the boundary layer revisions. The OH pure rotation \( 0 - 0 \) and H\(_2\)O lines are strengthened over the predictions from the MARCS model in such a way that the observed lines are well fit.

A lowering of the boundary layer temperatures of Arcturus was proposed by Wiedemann et al. (1994) who analyzed high-resolution spectra of CO fundamental vibration-rotation lines at 4.6 \( \mu m \). To explain the line depths of the strongest CO lines, Wiedemann et al. discarded a chromospheric temperature rise (which starts off at \( \tau_{500} \sim -3 \)) and required the boundary temperature to fall to 2400 K in the highest layers contributing the CO line cores. Their synthetic spectra were computed on the assumption of non-LTE for the excitation of the CO molecule. The temperatures in the boundary layer needed to fit the CO line profiles are dependent on the choice of (poorly known) collision cross-sections needed in the non-LTE calculation. For this and other reasons (e.g., we assume the OH and H\(_2\)O molecules are in LTE), quantitative agreement between the temperature profile in Figure 7 and the CO-based result is not expected. The boundary temperatures we derive are a few hundred degrees lower, but our model predicts the CO lines at 4.6 \( \mu m \) just as well.

The revisions to the upper boundary layer made by us were made solely with the aim of fitting observed line profiles. Here, we comment briefly on possible physical processes behind
a cooling of the boundary layer.

How accurately are the boundary layer temperatures predicted by the MARCS code? Assuming the underlying assumptions are valid, we may break the sources of uncertainty into two classes: those related to the defining atmospheric parameters, and those associated with the atomic and molecular data, principally the line blanketing. The atmospheric parameters of Arcturus are quite well determined based on a range of different observing techniques. No obvious source of line blanketing is discarded from the model calculation. However, there may be uncertainties in the input data.

The numerical uncertainties are certainly less than 50 K. One aspect of the statistical uncertainties in the modelled temperature structure may be estimated by selecting different numbers of points of the opacity sampling (OS) in the model calculation. The outer-most layers of the model will be sampled only by CO bands and the strongest metal lines. The temperature difference between using 2,100 and 11,000 OS points is at most 30 K and in the outer layers at most 10 K. Similarly, between using 2,100 and the full 84,000 OS points, the maximum difference in the temperature structure is 40 K, and in the most shallow parts also 10 K.

Relaxation of the assumptions behind the MARCS models may also change the atmospheric structure. Even small alterations of the heating or cooling terms in the energy equation (for example due to dynamic processes or uncertainties and errors in the calculations of radiative cooling) may lead to changes in the temperature structure in the outer, tenuous regions of the photosphere where the heat capacity per volume is low. The assumption of LTE is one target of model builders seeking to go beyond the standard assumptions. Atomic – continuous and line – opacity was treated in non-LTE using large model atoms by Short et al. (2002, in preparation) in spherical geometry, hydrostatic equilibrium, and flux constancy. Introduction of non-LTE in place of LTE lowered the boundary temperature by an amount quite similar to our empirical cooling of the MARCS model. This suggests that non-LTE effects in atoms may suffice to account for the surprising presence of H\textsubscript{2}O molecules in the photosphere.

5.2. An Inhomogeneous Atmosphere?

A key assumption made in construction and application of the model atmosphere is that physical conditions are everywhere the same at a given geometrical depth. Such a model is said to be ‘homogeneous’. Arcturus, with its deep convective envelope, is certain to be inhomogeneous, that is to exhibit surface granulation (Schwarzschild 1975) which may be
crude a characterization of consisting of columns of warm rising and cool sinking gas. The continuum intensity contrast in the mid-infrared will be small. There will, however, most likely be a sharp difference in the H$_2$O column density with the sinking column much richer in the molecules, and, as a result, the surface-averaged spectrum will show stronger H$_2$O lines than the spectrum of the equivalent homogeneous model atmosphere. Unfortunately, inhomogeneous model atmospheres of giant stars are unavailable, but we note that progress is being made (Freytag 2001). Yet, the modest 300 K cooling imposed on the MARCS model is surely within the range of temperature differences between rising and sinking granules. Note that granulation is likely to have a weaker effect on the CO lines because carbon atoms are quite fully associated into CO molecules. Contrast between the CO column density for the rising and sinking granules will be less than for H$_2$O.

An alternative mechanism for producing inhomogeneities is variously known as ‘a molecular catastrophe’ or ‘temperature bifurcation’. In warm stars, the CO molecular opacity influences the temperature profile predicted by a program like MARCS. If the temperature of gas in the boundary layer is perturbed, there may be a runaway to one of two different solutions. Suppose the gas is cooled, more CO molecules form and increase the cooling of the boundary layer. The temperature drop leads to yet more CO molecules and to a runaway to a ‘cool’ boundary layer. Conversely, if the perturbation raises the temperature, CO molecules are dissociated, the cooling rate decreased, and the temperature rise is continued. In cool O-rich stars, where the CO number density is limited by the abundance of carbon, this sensitivity of opacity to temperature is greatly reduced, but other molecules (e.g., SiO or H$_2$O) may act in a similar way. Quite detailed studies of the bifurcation induced by CO molecules have been made for the Sun and similar stars (Muchmore & Ulmschneider 1985; Muchmore 1986; Muchmore et al. 1988). Supporting evidence has come from observations of CO 4.6 $\mu$m lines at high spectral resolution (Ayres & Testerman 1981; Ayres et al. 1986). Convective velocity flows are likely to hamper the development of the temperature bifurcations (Steffen & Muchmore 1988).

Arcturus certainly exhibits a chromosphere, which has been modelled by Ayres & Linsky (1975). Limits on its filling factor are discussed by Wiedemann et al. (1994) based on their deduced temperature structure. It is suggested that the hot component can not be larger than few percent. Existence of the chromosphere around Arcturus suggests a heating mechanism active in and above the upper photosphere. Cuntz & Muchmore (1989) made a preliminary study of the effects of propagating acoustic waves including molecular line cooling. When the waves lead to weak shocks, a cool atmosphere is formed: temperatures as low as 1000 K were predicted. These temperatures are substantially below those required to account for the H$_2$O lines and the CO 4.6 $\mu$m lines (Wiedemann et al. 1994). On the other hand, strong shocks lead to a temperature inversion, approximately matching an empirical
5.3. Non-LTE Effects

Order of magnitude estimates of collisional and radiative rates indicate that the vibronic structure of the OH and H$_2$O molecules are unlikely to be in LTE throughout the boundary layer. To illustrate this claim, we compare rates of de-excitation through collisions and photons.

Collisional de-excitation occurs at a rate $C_{ul} \sim N_H \sigma_{ul} v_{rel}$ where we consider H atoms at density $N_H$ to be the dominant collision partner, the cross-section $\sigma_{ul}$ is taken as the geometrical area ($\sim 10^{-15}$ cm$^{-2}$), and $v_{rel}$ is the relative velocity between the H atom and the molecule ($\sim 5$ km s$^{-1}$). To maintain LTE a minimum condition is that the rate $C_{ul}$ must exceed the rate of spontaneous emission given by sum of the Einstein coefficients ($A_{ul}$) from the upper level. For the OH molecule, the $A$-values of rotational levels of the lowest vibrational level ($v' = 0$) run from about $2$ s$^{-1}$ at low $J$ to about $1000$ s$^{-1}$ at $J \simeq 40$ scaling approximately as $J^2$ (Goldman et al. 1998). For other vibrational levels, the values are of a similar magnitude even when the contribution of vibration-rotation transitions are included in the deexcitation. A-values of the H$_2$O levels, for the lines of interest, range from 10 to 1000 s$^{-1}$.

Supposing the sum of the $A$ values to be $A_{sum} = 1$, 100, and 1000 s$^{-1}$, $C_{ul} \sim A_{sum}$ for gas pressures $\log P_g \sim -3.2$, $-1.2$, and $-0.2$ (cgs) which according to Fig. 7 correspond, for the first value, to an optical depth beyond our boundary point, and for the second and third ones, to $\log \tau_{500} \sim -6$ and $-5$, respectively. For example, for the water-vapor line at $818.4$ cm$^{-1}$, with an $A_{ul}$ of 600 s$^{-1}$, we find a critical gas pressure of $\log P_g \sim -0.4$ (cgs) which occurs already at $\log \tau_{500} \sim -5.3$. Hence, we cannot be confident that collisions will dominate over radiative decay and therefore we can not conclude, on the basis of this calculation, that LTE necessarily prevails for the line formation in the very outer layers of the photosphere. The effect on line depths is difficult to determine. A proper non-LTE calculation is necessary to determine whether LTE does in fact prevail and what the effects would be due to a departure from LTE. To complete the assessment of non-LTE effects, one should study the chemistry, that is the radiative and collisional processes controlling the density of OH and H$_2$O molecules. In general, these rates are expected to be lower than those controlling the excitation.
6. CONCLUDING REMARKS

We have made an unexpected discovery of absorption lines of water vapor in the disk-averaged spectrum of Arcturus. Based on kinematic information, line widths and excitation temperature, we argue that the water vapor is photospheric and not circumstellar. Until now, H$_2$O has not been expected to exist in photospheres of stars of Arcturus’ effective temperature. This is true unless the outer layers of the model photosphere do not describe these regions properly. By modifying these layers we have succeeded in finding a model which yields a synthetic spectrum matching the observations. We are, however, not claiming that this necessarily is the only and true model. Our exercise simply shows that it is possible to achieve a photospheric spectrum containing water vapor also for early K giants if the outer parts are cooled for some reason. Possible reasons for the unexpected water vapor include photospheric inhomogeneities (such as convective flows, molecular catastrophes, or even star spots) and departures from LTE in the photospheric structure or line formation in the boundary layers.

We note that it is obvious that the chromospheric model proposed for Arcturus (Ayres & Linsky 1975) would not fit our mid-infrared observations. This circumstance was also found by Wiedemann et al. (1994) analyzing near-infrared CO data. Wiedemann et al. conclude that the upper photosphere has to be inhomogeneous with a quiet and a chromospheric part. Perhaps, the chief challenge reinforced by our detection of water vapor concerns development of tools with which to construct empirical atmospheres of an inhomogeneous atmosphere. The mid-infrared H$_2$O and OH lines, also the cores of the 4.6 µm vibration-rotation lines, are useful probes of the cooler gas in the upper photospheric layers. Ultraviolet emission lines may be the best probe of the hotter gas in these (and higher) layers. What happens at several scale heights above these layers? One possibility is that deposition of mechanical energy heats the cool upflowing gas and largely erases the distinction between ‘hot’ and ‘cool’ gas. With the drop in density and the concomitant increase in cooling times, the gas may remain warm to very large distances from the red giant.

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