INFRARED SPECTRA AND VISIBILITIES AS PROBES OF THE OUTER ATMOSPHERES OF RED SUPERGIANT STARS

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ABSTRACT

In the light of the recent results of the stellar interferometry, we examine the nature of the extra molecular layer outside the photosphere of red supergiant stars, so far studied mostly with the use of the infrared spectra. Although the visibility data are more direct probes of the spatial structure of the outer atmosphere, it is essential that they are analyzed in combination with the spectral data. In the case of the M2 supergiant \( \mu \) Cephei, several sets of data, both spectra and visibilities, strongly suggested the presence of an extra molecular layer (which we referred to as “MOLsphere” for simplicity), and the basic parameters of the MOLsphere are estimated to be excitation temperature \( T_\text{ex} \approx 1600 \text{ K} \), column densities of CO and H\(_2\)O molecules \( N_\text{col} \approx 3.0 \times 10^{20} \text{ cm}^{-2} \), and located at about one stellar radius above the photosphere or \( R_{\text{ex}} \approx 2.0R_* \). The result shows reasonable agreement with the one based on the infrared spectra alone, and the model inferred from the spectra is now fully supported with the recent visibility data. In the case of the M2 supergiant \( \alpha \) Orionis, the infrared spectra and visibilities show a consistent picture in that its MOLsphere is closer to the photosphere (\( R_{\text{in}} \approx 1.3R_* \)) with higher gas temperature (\( T_{\text{ex}} \approx 2250 \text{ K} \)) and lower gas column density (\( N_\text{col} \approx 10^{20} \text{ cm}^{-2} \)), compared with that of \( \mu \) Cep. Some controversy on the interpretation of the mid-infrared data of \( \alpha \) Orionis can be reconciled. Given that the presence of the extra molecular layer is reasonably well established, the major unsolved problem is how to understand the origin of such a rather warm and dense layer in the outer atmosphere.

Subject headings: molecular processes — stars: individual (\( \alpha \) Ori, \( \mu \) Cep) — stars: late-type — supergiants

1. INTRODUCTION

Detailed studies on the structure of the outer atmospheres of cool luminous stars started with high-resolution infrared spectroscopy. Especially, Fourier transform spectroscopy (FTS) pioneered by P. and J. Connes (e.g., Connes 1970) and developed at Kitt Peak National Observatory (KPNO; Hall et al. 1979) played a major role for this purpose (e.g., Ridgway & Brault 1984). The possible presence of an extra molecular layer distinct from the cool expanding wind and from the hotter chromosphere was first noticed in Mira variables whose spectra of the CO 2–0 band showed extra absorption that remained stationary against the velocity shift of the photospheric lines due to pulsation (Hinkle et al. 1982). In the case of red supergiant stars, subtle excess absorption seen on the high-resolution FTS spectra of the CO first-overtone bands was interpreted as due to a quasi-static molecular layer above the photosphere (Tsuji 1987). The presence of the strong photospheric absorption lines of CO, however, made it rather difficult to be fully convinced of such a result.

In hindsight, more clear evidence for the presence of the extra molecular layers was observed with the balloon-borne IR telescope, known as Stratoscope II, at the infancy of the infrared astronomy in the early 1960s by Woolf et al. (1964) and Danielson et al. (1965), who have correctly identified water vapor spectra in several early M giant and supergiant stars. Later, it was recognized that the Stratoscope data should be more convincing evidence for the extra molecular layers, since water cannot be formed in the photospheres of these early M giant and supergiant stars (Tsuji 2000a). Also, another space IR observation by Russell et al. (1975), which showed flux excess in the 5–8 \( \mu \)m region of \( \mu \)Cephei, was interpreted as due to the thermal emission of water in the circumstellar envelope (Tsuji 1978a). The next major progress was provided by the Infrared Space Observatory (ISO) mission launched in 1995 (Kessler et al. 1996), and ISO uncovered that water exists everywhere in the universe, including the early M giant stars (e.g., Tsuji et al. 1997a; Decin et al. 2003). Finally, water was found in emission in the 6–7 \( \mu \)m region as well as in the 40 \( \mu \)m region of \( \mu \) Cephei observed with the Short Wavelength Spectrometer (SWS) (de Graauw et al. 1996) on board ISO, and the extraphotospheric origin of water lines appeared to be more likely (Tsuji 2000b).

The problem of water in cool stars, however, may involve some other aspects. Especially, water vapor lines were detected on the high-resolution 12 \( \mu \)m spectrum of the K giant star \( \alpha \) Boo by Ryde et al. (2002), who suggested that this result can be explained as due to an anomalous structure of the photosphere. Since it is not likely that such an early K giant star could have an extra molecular layer, it may be difficult to apply the “MOLsphere” scenario to this case. More recently, water vapor lines were clearly observed in the 12 \( \mu \)m region of \( \alpha \) Ori by Ryde et al. (2006), who argued the possibility of the photospheric origin as in the case of \( \alpha \) Boo. This observation confirmed the previous detection of the pure rotation lines of H\(_2\)O in \( \alpha \) Ori and \( \alpha \) Sco by Jennings & Sada (1998), who suggested that the water lines may be formed in the temperature minimum region of the photosphere-chromosphere transition. Thus, to understand the full meaning of water spectra in cool stars (but not necessarily very cool such as Mira variables and IR stars), more works on cool stellar atmosphere, including the photosphere, chromosphere, and outer molecular layer, should be required.

For more detailed analysis of the structure of the extra molecular layers, direct information on the spatial structure should be indispensable. Direct evidence for the presence of the extended molecular envelope was first given for Mira variables \( \alpha \) Ceti and R Leo with the Speckle interferometry by Labeyrie et al. (1977), who showed that the angular diameters in the region strongly blanketed by the TiO bands are larger by 2 times than those in the region free from the TiO bands. In normal M giants and especially in M supergiants, the angular diameters in the TiO bands relative...
to those outside of the TiO bands were found to be larger by as much as 20% by Quirrenbach et al. (1993), who pointed out that such an effect should not necessarily be related to the stellar pulsation and hence may be a more fundamental property of cool luminous stars. Recently, multiwavelength measurements of the angular diameters are extended to the infrared region, including the $K$ band (Dyck et al. 1992, 1996, 1998; Perrin et al. 2004a), $L'$ band (Chagnon et al. 2002; Mennesson et al. 2002), and mid-infrared (Weiner et al. 2003). For the case of $\alpha$ Ori, the resulting apparent diameter at 11 $\mu$m is $\approx$30% larger than that at the $K$ band, while the $L'$-band diameter showed little difference from the $K$-band diameter. These results can be interpreted as due to the differences of the atmospheric extensions due to the variations of the opacities with wavelength.

More recently, multiwavelength spatial interferometry with four narrowband filters within the $K$ band has been done for $\mu$ Cep by Perrin et al. (2005). Such an observation is what we have been looking for a long time and should be regarded as a milestone toward the ultimate observations with high resolution in both the spectral and spatial domains. Thus, such an observation can be expected to provide a final confirmation of the molecular layers outside the photosphere by showing direct evidence for the dependence of the geometrical extensions on the molecular opacities. We had to know, however, that the situation is by no means so optimistic: the MOLsphere viewed with the visibility data by Perrin et al. (2005) is characterized by the radius of about 1 R$_e$ and excitation temperature near 2700 K, while that viewed with the infrared spectra is characterized by the inner radius of about 2 R$_e$ and temperature about 1500 K (Tsuji 2000b). Clearly, the discrepancies are too large to be attributed to the uncertainties of the observations, and we investigate in this paper if a more consistent solution can be obtained from the spectral and visibility data.

Even for the case of $\alpha$ Orionis, which has been a target of extensive observations with a wide spectral coverage and with a variety of methods, our picture of its outer atmosphere appears to have not fully converged yet. An extreme case is the water absorption lines observed with a high resolution around 12 $\mu$m by Ryde et al. (2006), who attributed the origin of the observed H$_2$O lines to the anomalies of the photospheric structure rather than of the outer atmosphere, as already noted before. Such an interpretation is apparently against the recent interferometric observations (Weiner et al. 2003; Perrin et al. 2004a) and the detailed analyses of the visibility data together with the spectroscopic data (Ohnaka 2004; Verhoe St et al. 2006). Such a controversy may be a manifestation of the extreme complexity of the outer atmosphere of Betelgeuse and hopefully is a clue to further progress.

2. METHOD OF ANALYSES

Currently, we have no method of treating the outer atmospheres of cool luminous stars consistently. Under such a situation, we introduce an ad hoc model just to provide a frame by which numerical analysis such as of the spectra and visibilities can be done.

2.1. Basic Stellar Parameters

As a boundary condition to the outer atmosphere, we use the classical spherically extended LTE model photospheres in radiative and hydrostatic equilibrium. The basic parameters we have applied are summarized in Table 1. We keep most of the basic parameters of the photosphere we have used before (Tsuji 2000a, 2000b). It is true that even the effective temperatures of red supergiants are not yet well established, and there is no definitive answer at present. We assumed $T_{\text{eff}} = 3600$ K for $\alpha$ Ori, which is consistent with the recent interferometry determinations (Dyck et al. 1992, 1996, 1998; Perrin et al. 2004a). We changed $T_{\text{eff}}$ of $\mu$ Cep to 3800 K for the reason to be discussed in § 3.2. The effect of $T_{\text{eff}}$ on the predicted infrared spectra can be seen by comparing Figures 2b and 3b, for example.

The CNO abundances are most important, since they give a direct effect on the infrared spectra. We reanalyzed the equivalent width data of OH and NH measured on the FTS spectra of Betelgeuse by Lambert et al. (1984) with our model photosphere of $T_{\text{eff}} = 3600$ K, and we confirmed the N and O abundances for $\alpha$ Ori, which shows $T_{\text{eff}} = 3600$ K determined by Lambert et al. (1984), who analyzed the effect of $T_{\text{eff}}$ on the derived CNO abundances. As for the C abundance, we analyzed some weak lines of the CO first-overtone bands measured from the high-resolution FTS spectra and our C abundance, as shown in Table 1, is a factor of 2 smaller than the value of $\log (A_{C}/A_{H}) \approx -3.7$ (for $T_{\text{eff}} = 3600$ K) by Lambert et al. (1984). The major motivation to have reanalyzed the carbon abundance is the poor fits of the CO features at 1.7 and 2.3 $\mu$m regions in our previous Figures 2 and 3 (Tsuji 2000a). With our new C abundance, fits in these regions are considerably improved as can be seen in Figures 2b–4b, 7b, and 9a–12a. The micro- and macroturbulent velocities are also found from the same analysis and will be discussed elsewhere with details on the abundance analysis (T. Tsuji 2006, in preparation). The abundance analysis is more difficult for $\mu$ Cep, which shows very broad lines, and we assume the same abundances as for $\alpha$ Ori.

2.2. Model Photospheres

Our model photosphere code is essentially the same as our previous one (Tsuji 1976), except that the photosphere is now assumed to be spherically symmetric rather than plane-parallel. Also opacity data are updated (see the Appendix of Tsuji 2002a). We are including the radiation pressure $P_{\text{rad}}$ and turbulent pressure $P_{\text{turb}}$ in the hydrostatic equilibrium, and thus

$$\frac{1}{\rho} \frac{dP_{\text{gas}}}{dr} = -g_{\text{eff}},$$

(1)

where $\rho$ is the density, $P_{\text{gas}}$ is the gas pressure, and

$$g_{\text{eff}} = g_{\text{grav}} - g_{\text{rad}} - g_{\text{turb}},$$

(2)

with

$$g_{\text{grav}} = G \frac{M}{r^2},$$

(3)

$$g_{\text{rad}} = \frac{4\pi}{c} \int_0^\infty \kappa_\nu \pi F_\nu \, d\nu,$$

(4)
and

\[ g_{\text{tur}} = - \frac{1}{\rho} \frac{dP_{\text{tur}}}{dr}. \]

The notations have their usual meanings, and we assume \( P_{\text{tur}} = \rho \mathcal{C}_v^2 \), with the turbulent velocity \( \mathcal{C}_{\text{tur}} \). The photosphere is stable as long as \( g_{\text{tur}} > 0 \), and this stability limit was defined as the “Eddington limit” for the turbulent plus radiation pressure by De Jager (1984), in analogy with Eddington’s well-known stability limit for the radiation pressure.

Usually, integration of the model photosphere starts at a very small optical depth in the continuum (or optical depth in the mean opacity, e.g., Rosseland mean optical depth \( \tau_R \)) such that \( \tau_0 = 10^{-6} \). For \( T_{\text{eff}} = 3600 \, \text{K} \) and for the other parameters in Table 1, the photosphere extends to \( r(\tau_0 = 10^{-6}) \approx 730 \, R_\odot \) with \( r(\tau_0 = 1) \approx 650 \, R_\odot \), as shown by the solid lines in Figure 1. However, it is possible to construct a highly extended model photosphere in radiative and hydrostatic equilibrium, just starting at a still smaller optical depth within the stability limit noted above. An example starting at \( \tau_0 = 10^{-14} \) (again \( T_{\text{eff}} = 3600 \, \text{K} \), and other parameters in Table 1) is shown by the dashed lines in Figure 1. The photosphere expands to \( r(\tau_0 = 10^{-14}) \approx 1700 \, R_\odot \) for this case, again with \( r(\tau_0 = 1) \approx 650 \, R_\odot \). Thus, within the framework of the classical model photospheres, a model photosphere can be extended, at least formally, to as large as a few stellar radii due to the radiation and turbulent pressures. However, it is to be noted that such a model should not be regarded as physically realistic. In fact, the basic assumption such as LTE should certainly not be applied at a density as low as \( 10^{-20} \, \text{g cm}^{-3} \) (see Fig. 1). For this reason, such a model will not be used in our actual analysis, but only as a reference for an ad hoc model of the MOLsphere to be discussed in § 2.3.

If we start the integration from a still smaller optical depth or if we assume a somewhat larger turbulent velocity, the photosphere can no longer stay within De Jager’s generalized Eddington limit and expands without limit. Our purpose here is not to investigate such a stability limit, but we hope that such an extended photosphere may give some clues for modeling the MOLsphere. Unfortunately, however, the matter included in the extended part (e.g., outside of \( \tau_0 \approx 10^{-6} \)) is very small and has little effect on the spectra and the visibilities. It is difficult to deposit more matter in the upper photosphere within the framework of the hydrostatic equilibrium model, even though that kind of dynamical effect is introduced through the turbulent pressure. One idea may be to consider some kind of shock wave by which the rarefied gas can be compressed and heated (e.g., Woitke et al. 1999), and the extended photosphere can provide the preshock condition for such a model.

2.3. Ad Hoc Model of the MOLspheres

We recognize that it is difficult to construct a self-consistent model of the MOLsphere at present, and we use an ad hoc model starting from the extended photosphere discussed in § 2.2. We consider a model of MOLsphere specified with the excitation temperature \( T_{\text{ex}} \), gas column density \( N_{\text{col}} \), and inner radius \( R_{\text{in}} \). Then, in the layers above \( r = R_{\text{in}} \) in the extended LTE photosphere, the temperatures are replaced with \( T_{\text{ex}} \) and the matter densities are increased by a factor \( N_{\text{col}}/N_{\text{LTE}} \), where \( N_{\text{LTE}} \) is the LTE column density of the extended photosphere above \( r = R_{\text{in}} \). The resulting molsphere is isothermal at \( T_{\text{ex}} \), with the column density \( N_{\text{col}} \), and extending between \( r = R_{\text{in}} \) and the outer radius \( r = R_{\text{out}} \), which is near that of the starting extended photosphere (e.g., \( R_{\text{out}} \approx 1700 \, R_\odot \) if starting from the model of Fig. 1). Since the matter density is rather high near the inner radius, the effect of the outer radius is not important, but outer radius can be changed, if necessary, by starting from the extended photospheric model with different \( \tau_0 \). The matter densities and temperatures below \( R_{\text{in}} \) conserve the original LTE values of the extended photosphere, but they have little effect on the resulting spectra and visibilities because the matter densities there are very low.

Our model of the MOLsphere is not a physical model at all, and no longer in radiative and hydrostatic equilibrium, but will be used as a means by which to compute spectra and visibilities and to infer the physical parameters such as temperature, column density, and size of the MOLsphere from the observed data. This model is essentially the same as just assuming an envelope or shell of given parameters, as is usually done. An advantage of our formulation is that the spectral synthesis and related computer codes being used for the photospheres can directly be used for our MOLsphere plus photosphere models with almost no changes.

2.4. Spectra and Visibilities

We compute the specific intensity \( I_\nu(\mu) \) with our spectral synthesis code for 98 values of \( \mu \), where \( \mu = \cos \theta \) (\( \theta \) is the angle between the normal and the direction to the observer). Then, the flux \( F_\nu(\tau) \) is given by

\[ F_\nu(\tau) = 2 \int_0^1 \mu I_\nu(\mu) d\mu = 2 \sum_{i=1}^{98} w_i \mu_i I_\nu(\mu_i), \]

\[ \text{Note that } R_{\text{out}} \text{ differs in the models to be discussed below (models A–H in Tables 2 and 4) even for the same starting extended photosphere, and this is because the hydrostatic equilibrium is solved in each starting model with the isothermal MOLsphere of different } T_{\text{ex}}. \text{ These computations, however, are to determine } N_{\text{LTE}} \text{ needed to estimate } N_{\text{col}} \text{ rather than to evaluate } R_{\text{out}}. \]
with the abscissa \( \mu \), and weight factor \( w_i \) for Gaussian integration. Then, \( F_\nu^v(r) \) corrected for the dilution effect is obtained by

\[
F_\nu^v(r) = r^2 F_\nu(r)/R_e^2,
\]

where \( R_e \) is the stellar radius at \( \tau_R \approx 1 \) and defines the effective temperature \( T_{\text{eff}} \) through \( L_* = 4\pi R_e^2 \sigma T_{\text{eff}}^4 \) (\( L_* \) is the stellar luminosity and \( \sigma \) is the Stefan-Boltzmann constant).

The spectra are computed with the resolving powers of \( 5 \times 10^4 \)–\( 10^5 \) and convolved with the slit functions matching to the resolutions of the observed spectra. We use the line list including \( \text{H}_2\text{O} \) (Partridge & Schwenke 1997), OH (Jacquinet-Husson et al. 1999), CO (Guelachivili et al. 1983; Chackerian & Tipping 1983), SiO (Lavas et al. 1981; Tipping & Chackerian 1981; Langhoff & Bauschlicher 1993), and CN (Cerny et al. 1978; Bauschlicher et al. 1988). All of these molecular species (\( \text{H}_2\text{O}, \text{OH}, \text{CO}, \text{SiO}, \text{CN} \)) are included in the calculation of photospheric spectra, but only \( \text{H}_2\text{O} \) and CO are included in the MOLsphere.

For a spherically symmetric object with radius \( R \), the visibility \( V_* \) is obtained through the Fourier transform of the strip intensity distribution, \( \Phi_\nu(x) \), defined by

\[
\Phi_\nu(x) = 2 \int_0^{\sqrt{R^2-x^2}} I_\nu(x, y)dy,
\]

where \( I_\nu(x, y) \) is the intensity at \((x, y)\) on the object surface and the baseline of the interferometer is in the \( x \)-direction (Michelson & Pease 1921). In the numerical analysis of the extended envelope around the central star, we follow the formulation we have used before (Tsuji 1978b): we introduce

\[
p = \frac{x}{d/\theta_e/2},
\]

where \( \theta_e \) and \( d \) are the angular diameter of the central star and distance to the object, respectively, and

\[
v = \frac{1/\lambda}{\theta_e/2},
\]

where \( l \) and \( \lambda \) are the separation of the two telescopes on the interferometer baseline and wavelength, respectively. Then, the monochromatic visibility \( V_\nu \) is given by

\[
V_\nu(\nu) = \frac{\int_0^\infty \Phi_\nu(p) \cos(2\pi \nu p)dp}{\int_0^\infty \Phi_\nu(p)dp},
\]

For comparison with observed visibilities, which are usually obtained through broadband or narrowband filters, the monochromatic visibilities are squared and averaged with the filter transmissions as weights to have the band-averaged visibility, following Perrin et al. (2004a).

3. THE M SUPERGIANT STAR \( \mu \) CEPHEI

With the use of the recent visibility data, we first examine our previous model of the MOLsphere of \( \mu \) Cep based on the infrared spectra alone (Tsuji 2000a, 2000b) and confirm that the model is already reasonably consistent with the recent visibility data (§ 3.1). We further show that the model can be revised to be more consistent with both the visibility and spectral data (§ 3.2). The resulting model, however, does not agree with the model based primarily on the visibility data (Perrin et al. 2005), and we show that the spectral data are as important as the visibility data in modeling the outer atmospheres of cool luminous stars (§ 3.3).

3.1. MOLsphere as Seen by the Infrared Spectra

First, we examine a model based on the parameters derived from the infrared spectra (Tsuji 2000a, 2000b), as summarized in Table 2 under model A. It is to be remembered that the temperature and column density were estimated from the width and depth of the \( \text{H}_2\text{O} \) 1.9 \( \mu \)m bands, respectively, on the Stratoscope spectrum. The inner radius was estimated from the strength of the \( \text{H}_2\text{O} \) 6.3 \( \mu \)m bands in emission on the ISO spectrum. Thus, our model consists of the photospheric model of \( T_{\text{eff}} = 3600 \) K and the MOLsphere model characterized by the excitation temperature \( T_{\text{ex}} = 1500 \) K, \( \text{H}_2\text{O} \) and CO column densities of \( N_{\text{col}} \approx 3.0 \times 10^{20} \) cm\(^{-2} \), and inner radius of \( R_{\text{in}} \approx 1300 \) \( R_\odot \) (\( \approx 2R_e \)). The MOLsphere, starting from the extended photosphere of Figure 1, actually extends from \( R_{\text{in}} \approx 1300 \) \( R_\odot \) to \( R_{\text{out}} \approx 1700 \) \( R_\odot \), but effective contribution comes from the layers close to the inner radius where the density is relatively high.

We now examine this model of the photosphere-MOLsphere with the recent visibility data for the four narrowband regions within the \( K \) band by Perrin et al. (2005). We compute the intensity \( I_\nu(\mu) \) at the spectral resolution of 0.1 cm\(^{-1} \) for our combined model of the photosphere and MOLsphere, and the strip intensity distributions and visibilities are evaluated, as outlined in § 2.4. We apply the angular diameter of the central stellar disk of \( \theta_e = 14.11 \) mas as estimated by Perrin et al. (2005). In evaluating the band-averaged visibility from the monochromatic visibilities, the filter transmission of each narrowband filter is approximated by the Gaussian with the parameters given in Table 1 of Perrin et al. (2004b). In comparing the predicted and observed visibilities, the \( \chi^2 \) value is evaluated by

\[
\chi^2 = \sum_{i=1}^{N} \left[ \frac{V_i(\text{obs})^2 - V_i(\text{model})^2}{\sigma_i} \right]^2,
\]
where $V_{i}(\text{obs})$ and $V_{i}(\text{model})$ are the observed and predicted visibilities, respectively, $\sigma_{i}$ is the error estimate to $V_{i}(\text{obs})$, and $N$ is the number of data points for each band.

The predicted visibilities based on model A are compared with the observed ones by Perrin et al. (2005) in Figure 2a. The fits are pretty good for the $K239$ band, which is strongly blanketed with the CO and H$_2$O lines [$\chi^2(K239) = 0.23$], and for the $K215$ band, which is relatively free from molecular lines [$\chi^2(K215) = 5.67$]. However, the fits are poor for the $K203$ band, which suffers the effect of the H$_2$O 1.9 $\mu$m bands [$\chi^2(K203) = 53.68$], and for the $K222$ band, which includes no known strong molecular bands [$\chi^2(K222) = 52.70$]. The poor fits in these bands are largely due to the higher predicted visibilities at the highest spatial frequencies compared with the observed ones. Thus, further fine-tunings in our modeling should be required.

The predicted near-infrared spectrum based on model A is compared with the Stratoscope spectrum in Figure 2b. In the following comparisons of the observed and predicted spectra, the observed data are shown by the filled circles and the predicted spectra by the solid lines in general. The ordinate scale always refers to the predicted spectrum (in units of the emergent flux from the unit surface area, i.e., in ergs cm$^{-2}$ s$^{-1}$ Hz$^{-1}$), to which the observed one is fitted. Also, the predicted spectrum from the photosphere is shown together with that from the MOLsphere plus photosphere in most cases. The details of the Stratoscope spectra and the ISO spectra were discussed before (Tsuji 2000a, 2000b), and all of the spectra of $\mu$ Cep are dereddened with $A_V = 1.5$ mag.

This comparison of the Stratoscope spectra with the predicted ones has already been done before (Tsuji 2000a), but some improvements have been made since then. First, the extra molecular layer was approximated by a plane-parallel slab in the previous analysis, and this was thought to be a reasonable approximation for the near-infrared. However, the result based on the spherical MOLsphere shown in Figure 2b reveals that the sphericity effect is already important in the near-infrared. This is clearly seen in the CO first-overtone bands around 2.5 $\mu$m, whose excess absorption was too large in the previous analysis (see Fig. 3 of Tsuji 2000a) compared with the present result in Figure 2b. This is because the emission in the extended MOLsphere already has significant contribution to the integrated spectrum. The predicted CO absorption around 2.5 $\mu$m, however, still appears to be deeper compared with the observed one. So far, we assumed that the column density estimated from the H$_2$O features applies to CO as well, but it may be possible that the CO column density is somewhat smaller. However, we assume that the column densities for CO and H$_2$O are the same for simplicity.

Second, the region of the CO second-overtone bands around 1.7 $\mu$m, which was depressed too much compared with the observation in our previous analysis (Fig. 3 of Tsuji 2000a), is now improved in Figure 2b, and this is the effect of the revised carbon abundance noted in § 2.1. Also, the improved fit near 2.5 $\mu$m is partly due to the revision of the carbon abundance as well. As a result, the near-infrared spectrum observed by Stratoscope including the H$_2$O 1.4 and 1.9 $\mu$m bands can be well matched with our prediction based on model A. Although the observed flux shortward of 1.3 $\mu$m shows some excess compared to the prediction, this may be a problem of the photospheric spectrum, which is also shown in Figure 2b and shows only CO and CN bands.

The predicted spectrum in the H$_2$O $\nu_2$ band region based on model A is compared with the ISO spectrum in Figure 2c. This comparison has also been made before with the use of the spherically extended MOLsphere model$^5$ (Tsuji 2000b), but we now use the H$_2$O line list by Partridge & Schwenke (1997) instead of the HITTEMP database (Rothman 1997$^4$) used before. The tendency that the H$_2$O $\nu_2$ bands appear in emission can be well reproduced with our model A, but the predicted emission is still not strong enough to explain the observed spectrum in the region around 6.8 $\mu$m. The predicted spectrum based on the model photosphere appears at the lower left corner.

$^3$ This model was a preliminary version of model A and not exactly the same as it.

$^4$ Available at http://www.cfa.harvard.edu/hitran.
possibilities 1 and 2 systematically by changing the temperature.

Also, since the visibilities based on model A are already consistent with the near-infrared spectrum and we do not consider possibility 3 further. However, the column density is already well consistent with the observations at K215 and K239 bands, possibilities 1 and 2 must be considered so that the good fits in the visibilities already achieved can be conserved. We examine possibilities 1 and 2 systematically by changing the temperature by a step of 100 K and the inner radius by a step of 0.1R., Also, as to the observed excess shortward of 1.3 μm, we notice that the recent angular diameter measurements suggested a higher effective temperature of 3789 K (Perrin et al. 2005), and we apply T_{eff} = 3800 K in all of the models to be discussed below, instead of 3600 K used in model A. The extended photosphere of T_{eff} = 3800 K, used as the starting model for the MOLsphere, is quite similar to the case of T_{eff} = 3600 K shown in Figure 1. First, we examine the effect of changing R_{in} from 2.0R. ≈ 1300 R_⊙ for model A, keeping T_{ex} = 1500 K. After some trial and error, we find that a case of R_{in} ≈ 2.2R. ≈ 1430 R_⊙ shows some improvements. First, the resulting predicted visibilities for the four narrowbroad regions are compared with the observed data in Figure 3a: the fits for the K203 and K222 bands are somewhat improved with \( \chi^2(K203) = 40.51 \) and \( \chi^2(K222) = 40.95 \), but still not very good. On the other hand, fits for the K215 and K239 bands remain reasonable with \( \chi^2(K215) = 4.66 \) and \( \chi^2(K239) = 13.61 \). The good fits in the visibilities for the K239 band with model A are somewhat degraded but still remain reasonable. Second, the predicted flux in the region shortward of 1.3 μm is increased as a result of changing T_{eff} of the photosphere from 3600 to 3800 K, and the fit in this region now appears to be reasonable as shown in Figure 3b. Finally, the observed and predicted spectra in the 6–7 μm region are compared in Figure 3c. The predicted emission around 6.8 μm increases appreciably, and it is now sufficiently large to account for the observed emission as shown in Figure 3c. We refer to this model as model B, and its major parameters are summarized in Table 2.

Although model B is considerably improved compared to model A, we examine another possibility of changing T_{ex} of the MOLsphere from 1500 K for model A while R_{in} remains 2.0R.. The resulting predicted visibilities for a case of T_{ex} = 1600 K are again compared with the observed ones in Figure 4a: the fits for the K203 and K222 bands are both improved compared to the results for model B, with \( \chi^2(K203) = 29.24 \) and \( \chi^2(K222) = 27.76 \). At the same time, fits for the K239 band are further degraded but still remain acceptable with \( \chi^2(K239) = 17.68 \). The fits for the K215 band remain fine with \( \chi^2(K215) = 4.52 \), and this result that the fits for the K215 band remain nearly unchanged may be a natural consequence that this band region is a good continuum window. We conclude that this model, to be referred to as model C, provides better fits to the observed visibilities compared to model B. The predicted near-infrared spectrum shown in Figure 4b shows almost no change from Figure 3b, and we confirm that the 1.4 and 1.9 μm absorption bands depend primarily on the column density, which is unchanged throughout. The predicted emission around 6.8 μm reasonably accounts for the observed emission as shown in Figure 3c. The major parameters of model C are summarized in Table 2.

We examined several other models around models B and C, but no significant improvements were obtained. For example, a case of increasing R_{in} to 2.1R., keeping T_{ex} = 1600 K, results in degrading the fits in visibilities, although fits in spectra remain nearly the same. A case of increasing T_{ex} to 1700 K, keeping R_{in} = 2.0R., also results in degrading the fits in visibilities, while fits in spectra remain nearly the same. If R_{in} is decreased to 1.9R, at T_{ex} = 1700 K, the fits in visibilities for the K222 band are somewhat improved compared to those for model C, but the predicted emission around 6.8 μm is reduced to the level of model A. On the other hand, if T_{ex} is decreased to 1400 K, R_{in} had to be

\[ \chi^2(K203) = 35.64, \quad \chi^2(K215) = 8.91, \quad \chi^2(K222) = 18.04, \quad \text{and} \quad \chi^2(K239) = 31.15. \]
increased to $2.2R$, to keep the reasonable fits for the spectra, but the fits for the visibilities are degraded appreciably.

We conclude that model C is a possible best model that reasonably accounts for both the observed visibilities and infrared spectra simultaneously, within the framework of our highly simplified MOLsphere model. It is encouraging that our model could reproduce the general tendency that the visibilities in the region with strong H$_2$O and/or CO bands ($K_{203}$, $K_{239}$) are lower than those in the region with less molecular absorption ($K_{215}$, $K_{222}$), in agreement with the observations, even though the fits are not very good for the $K_{203}$ and $K_{222}$ bands. This result implies that the MOLsphere model based on the infrared spectra alone is reasonably consistent with the visibility data not known at the time when the modeling was done. This may be because the infrared spectra already include some information on the spatial structure of the extended atmosphere. It is most important, however, that the model is now examined directly with the interferometry, which is a direct probe of the spatial structure of the astronomical objects.

3.3. MOLsphere as Seen by the Visibility Data

We notice, however, that the model parameters of our model C show significant differences with those derived from the visibility data by Perrin et al. (2005) themselves: their excitation temperature is near 2700 K compared with 1600 K of our model C, and their radius of the molecular layer is about $1.3R_*$ compared with the inner radius $2.0R_*$ of our model C. To investigate the origin of the differences, we think that it is useful to analyze their model in the same way as in our models. For this purpose, we refer to a model based on their parameters as model D. Since their molecular layer is assumed to be a thin shell, we design the model D in our formulation to be extending from $R_{in} = 2.0R_*$ to $R_{out} = 2.5R_*$, for which the initial extended photosphere starts at $A_v = 10^2$, and thus the effective location of the thin shell of model D is at about $r = 1.3R_*$.

The gas column densities were not provided in the model of Perrin et al. (2005), but a mean optical thickness for each narrow-band region was given. Accordingly, we transform their optical thickness at each filter band region to the column densities with the absorption cross sections of CO and H$_2$O evaluated from the line list mentioned in §2.4 and shown in Figure 5, where the high-resolution results are shown by the black lines, while the smeared out straight means are shown by the white lines. The resulting column densities summarized in Table 3 appear to be different for different bands, while they should be the same at least for $2.03, 2.15, and 2.22 \mu m$, in which H$_2$O is the major source of opacity. The column density of CO can of course be different from that of H$_2$O. We assume that the column densities of CO and H$_2$O for the $2.39 \mu m$ region are the same as in Table 3, just as an example. But the optical thickness of $3.93$ for the $2.39 \mu m$ region given by Perrin et al. (2005) is large enough to completely mask the photospheric spectra, and the column density corresponding to $\tau = 3.93$ should anyhow be very large.

The major parameters of model D are summarized in Table 2, and we can now proceed as in our models A–C with these parameters. The resulting visibilities are shown in Figure 6 together with the absorption spectra. The black line is by the high resolution ($R \approx 50,000$), and the white line is the straight mean opacity smeared out with the resolution $R \approx 1600$. (a) Same as (a), but for CO.

![Absorption cross section of H$_2$O at T = 2700 K](image-url)
with the observed data by Perrin et al. (2005). The predicted visibilities using the column densities as input parameters nearly reproduce the ones for the K215, K222, and K239 bands shown in Figure 1 of Perrin et al. (2005) using the effective optical thicknesses as input parameters. However, such an agreement cannot be found for the K203 band, and this means that the transformation of the mean optical depth to the column density could not be done correctly. We cannot understand the reason for this, but the H2O cross section at a temperature as high as 2700 K may not be found correctly. We cannot understand the reason for this, but the mean optical depth to the column density could not be found for the H2O band. For this reason, the fits for the K203 band are quite poor with $\chi^2(K203) = 47.93$. It is, however, possible to improve the fits in the K203 band by just changing the column density somewhat, and we find a reasonable fit with $\chi^2(K203) = 16.98$ for $N_{\text{col}}(\text{H}_2\text{O}) = 4.2 \times 10^{20} \text{ cm}^{-2}$ after a few trials and errors (see dotted line in Figure 6). If we can choose four values of the free parameter such as the mean optical depth or the column density for the four observed data, it is certainly possible to have good fits for all of the observed data. However, such fits cannot be regarded as justification of such a model as D, since the values of the column densities are so different for the different bands (see Table 3).

Since the column densities should be unique for the different bands, we modify model D so that $N_{\text{col}}(\text{H}_2\text{O}) = 2.8 \times 10^{20} \text{ cm}^{-2}$, just as an example, for all four narrowband regions. Then, to account for $\tau = 3.93$ of the K239 band, which includes CO and H2O, it turns out that $N_{\text{col}}(\text{CO}) = 9.3 \times 10^{23} \text{ cm}^{-2}$ with the absorption cross sections given in Table 3. For this modified model D, to be referred to as model D*, we first evaluate the visibilities, and the results are again compared with the observed data in Figure 7a. The fits are generally fair with $\chi^2(K203) = 17.78$, $\chi^2(K215) = 25.24$, $\chi^2(K222) = 14.21$, and $\chi^2(K239) = 30.45$. The fits for the K203 and K222 bands are better than those for model C, while the fits for the K215 and K239 bands are better in model C. Thus, it is difficult to decide which of model C or model D* is to be preferred from the visibility analysis alone.

An advantage of using the column density instead of the mean optical thickness is that the spectra can be evaluated for the same input parameters. The near-infrared spectrum for model D* is compared with the Stratoscope data in Figure 7b. The fit is rather poor and the other $N_{\text{col}}(\text{H}_2\text{O})$ values in Table 3 produce too weak or too strong H2O absorption bands. We also evaluate the spectrum in the 6–7 $\mu$m region for $N_{\text{col}}(\text{H}_2\text{O}) = 2.8 \times 10^{20} \text{ cm}^{-2}$ and compared with the ISO data in Figure 7c. The predicted spectrum still appears in absorption and cannot be matched with the observed one at all. The results are more or less the same for other values of $N_{\text{col}}(\text{H}_2\text{O})$ in Table 3.

In our fine-tunings in §3.2, we increased the temperature from 1600 to 1700 K and, at the same time, decreased the inner radius from 2.0$R_*$ to 1.9$R_*$, and we obtained reasonable fits to the observed visibilities. If we pursued a solution in this direction, we might increase the temperature further and decrease the inner radius at the same time. The resulting model might be similar to model D*, but we might reject such a case since such a high-temperature, small-size model might not explain the 6–7 $\mu$m emission as can be inferred from the result shown in Figure 7c.  

Furthermore, this result can be applied to the case that the straight mean opacity is a reasonable approximation as for the hot water vapor. Note that this result can no longer be applied to CO for which the straight mean opacity no longer describes the spectrum accurately.

### Table 3

| Wavelength (\(\mu\)m) | \(a\) | Molecule | \(\kappa\) (cm\(^{-1}\)) | \(N_{\text{col}}\) (cm\(^{-2}\)) |
|-----------------------|------|----------|---------------------|---------------------|
| 2.03                  | 0.22 | H2O      | 1.6 $\times$ 10\(^{-21}\) | 1.4 $\times$ 10\(^{20}\) |
| 2.15                  | 0.02 | H2O      | 4.5 $\times$ 10\(^{-22}\) | 4.4 $\times$ 10\(^{19}\) |
| 2.22                  | 0.07 | H2O      | 2.5 $\times$ 10\(^{-22}\) | 2.8 $\times$ 10\(^{20}\) |
| 2.39                  | 2.62 | H2O      | 8.0 $\times$ 10\(^{-22}\) | 3.3 $\times$ 10\(^{21}\) |
|                      | 1.31 | CO       | 4.0 $\times$ 10\(^{-22}\) | 3.3 $\times$ 10\(^{21}\) |

\(\tau\) Perrin et al. (2005).

\(a\) Read from Fig. 5.

\(\kappa\) The total optical depth of $\tau = 3.93$ by Perrin et al. (2005) is divided into $\tau$ (H2O) = 2.62 and $\tau$ (CO) = 1.31 so that the column densities of H2O and CO are the same.

\(b\) The fit can no longer be applied to CO for which the straight mean opacity no longer describes the spectrum accurately.

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**Fig. 6.**—Predicted band-averaged visibilities based on the monochromatic visibilities (solid lines) for model D ($T_\text{eff}$ = 3800 K, $T_\text{ex}$ = 2700 K, $R_\text{in}$ = 1.3$R_*$, and the optical thickness for the four narrowband regions given in Table 3). It is confirmed that the results for the K215, K222, and K239 bands based on the column densities estimated with the cross sections of the contributing molecular bands (Figure 5) reproduce the predicted visibilities based on the mean optical thicknesses (Figure 1 of Perrin et al. 2005). The results also agree with the observed visibilities for $\mu$ Cep by Perrin et al. (2005) shown by the filled symbols. But the result for the K203 band does not reproduce the result of Perrin et al. (2005) for $\log N_{\text{col}} = 1.4 \times 10^{20}$ cm\(^{-2}\) in Table 3 (solid line labeled “!”), but we find that reasonable agreements with the predicted and observed values by Perrin et al. (2005) can be obtained for $\log N_{\text{col}} = 4.2 \times 10^{20}$ cm\(^{-2}\) (dotted line).
same time, Betelgeuse is a quite complicated object, and how to interpret the observed data is still controversial at least partly. We show below that unexpected water lines observed in Betelgeuse may be difficult to explain by anomalies within the framework of the photospheric models (§4.1). On the other hand, the infrared spectra and visibility data consistently show the presence of the extra molecular layers and provide consistent estimations of their basic parameters (§4.2). In the mid-infrared region, some recent observations are subject to controversy, but we look for a possibility to relax such an issue (§4.3).

4. The Case of α Orionis

Betelgeuse is an object probably best observed with a variety of methods, and new observed data are still accumulating. At the same time, Perrin et al. (2005) did not consider the spectral data and might be led to the high-temperature, small-size model that might have satisfied the visibility data well.

We conclude that it is difficult to decide the unique solution for the MOLsphere model from the visibility data alone, and it is indispensible to apply the spectroscopic data at the same time to have some idea of the model of the stellar outer atmosphere. At the same time, it is difficult to have good fits to the observed visibilities at all of the spatial frequencies within the framework of the simplified uniform spherically symmetric models of the MOLsphere. Certainly, some details of the fine structure of the outer envelope should be considered to have better fits at higher spatial frequencies, and our present analysis is only a very initial stage in the interpretation of the visibility data.

4.1. Can a Cool Photosphere Explain the Infrared Spectra of Betelgeuse?

This is a question addressed recently by Ryde et al. (2006), who observed high-resolution spectra of Betelgeuse in the 12 μm region and suggested that the observed H2O lines can be interpreted with the anomalous structure of the photosphere rather than assuming the presence of the extra molecular layers. They showed that their high-resolution 12 μm spectra could be well fitted with the predicted ones based on the cool photospheric models. However, it can be shown below that the near-infrared spectra cannot easily be matched by an anomalous structure of the photosphere.

Ryde et al. (2006) suggested that the observed H2O pure rotational lines in Betelgeuse can be accounted for with the thermal structure approximated by the classical model photosphere of \( T_{\text{eff}} \approx 3250 \text{ K} \) and that their observations can be explained with a rather small H2O column density of \( N_{\text{col}} \approx 5 \times 10^{18} \text{ cm}^{-2} \). This is possible because the \( f \)-values of the H2O pure rotational lines are pretty large. In Figure 8a, the spectra of the H2O pure rotation lines predicted from the classical spherically extended model photospheres of \( T_{\text{eff}} = 2800, 3000, 3200, 3400, \) and 3600 K (\( M = 15 \text{ M}_\odot, R = 650 \text{ R}_\odot, \xi_{\text{micro}} = 5 \text{ km s}^{-1}, \xi_{\text{macro}} = 10 \text{ km s}^{-1} \) throughout) are shown. Thus, weak H2O pure rotational lines can be observed already at \( T_{\text{eff}} = 3600 \text{ K} \) and increasingly stronger toward the lower \( T_{\text{eff}} \) values. At \( T_{\text{eff}} \approx 3200 \text{ K} \), H2O lines can certainly be observed even if they are diluted by the silicate dust emission in Betelgeuse.

However, with such a small column density, it is not possible to explain the H2O 1.4 and 1.9 μm bands observed with Stratoscope II, since the \( f \)-values of the near-infrared H2O lines are 1–2 orders of magnitude smaller than those of the pure rotation lines observed in the 12 μm region. In Figure 8b we show the near-infrared spectra predicted from the same models as used for Figure 8a and reduced to the resolution of the Stratoscope observations. It can be confirmed that the H2O 1.4 and 1.9 μm bands cannot be seen in the models with \( T_{\text{eff}} = 3200 \text{ K} \) and higher but appear in the models of \( T_{\text{eff}} = 3000 \text{ K} \) and lower. It is clear that the H2O 1.4 and 1.9 μm bands seen on the Stratoscope spectra (Figs. 9a–12a) cannot be accounted for with the cool photosphere of \( T_{\text{eff}} \approx 3250 \text{ K} \). Ryde et al. (2006) argued that the photosphere of Betelgeuse can be very peculiar, but the relative behaviors of the near- and mid-infrared spectra should remain nearly the same as long as any peculiarity remains within the photosphere. We conclude that the near- and mid-infrared spectra cannot be consistently interpreted by a cool atmosphere within the framework of the classical model photosphere. On the other hand, Ryde et al. (2006) suggested a possibility of an inhomogeneous atmosphere with a cool component giving rise to the 12 μm water lines and a hot component giving rise to the near-infrared H2O bands. Such a possibility should hopefully be examined further with other arguments suggesting the inhomogeneity in red supergiant stars (§5.1).
4.2. Can a MOLsphere Explain the Infrared Spectra of Betelgeuse?

For Betelgeuse, we have assumed the presence of an extra molecular layer above the photosphere and estimated $T_{\text{ex}} = 1500 \pm 500$ K and $N_{\text{col}} = 10^{20}$ cm$^{-2}$ from the Stratoscope spectra based on a simple slab model (Tsuji 2000a). Also, we have suggested that the weak 6.6 $\mu$m absorption observed with ISO can be explained if the inner radius of the MOLsphere is $R_{\text{in}} \approx 1.5R_\odot$ (Tsuji 2000b). This result, however, was given without a detailed numerical analysis and may not be accurate enough. We now re-examine such a model of Betelgeuse in some detail with some improvements such as noted in the analysis of $\mu$ Cep. The observed spectra of Betelgeuse have been discussed in detail before (Tsuji 2000a, 2000b) and are reddened with $A_V = 0.5$ mag.

For this purpose, we recall that the near-infrared spectra observed with Stratoscope II are relatively free from the effect of spherical extension of the MOLsphere, and thus they are very useful probes of the column density and temperature. Especially, we believe that the column density of H$_2$O can be well fixed from the strengths of the 1.4 and 1.9 $\mu$m bands to be $N_{\text{col}} \approx 10^{20}$ cm$^{-2}$. We confirm that this result remains unchanged for possible values of $T_{\text{ex}}$ and $R_{\text{in}}$ in the spherically extended MOLsphere models. Then, although the H$_2$O 6.3 $\mu$m bands do not appear in emission but only in weak absorption in the case of $\alpha$ Ori, they can be used to constrain the extension of MOLsphere and to refine the temperature. Thus, the nature of the extra molecular layer can also be inferred from these infrared spectra alone as in the case of $\mu$ Cep. The result should further be examined in the light of the interferometric observations. For this purpose, we refer to the recent work by Perrin et al. (2004a), who suggested a 2055 K layer located at $0.33R_\odot$ above the photosphere from the visibility data at the $K$, $L$, and 11.15 $\mu$m bands.

We assume $T_{\text{eff}} = 3600$ K for the central star and start from the extended photosphere of Figure 1. We examine first the case of $T_{\text{ex}} = 1500$ K and systematically changed the inner radius $R_{\text{in}}$ of the MOLsphere from 1.3$r\odot$, approximately the radius of the molecular layer by Perrin et al. (2004a). The near-infrared spectrum can be fitted reasonably well for any values of $R_{\text{in}}$ up to $\approx 2R_\odot$, with $N_{\text{col}} = 10^{20}$ cm$^{-2}$, but the 6–7 $\mu$m spectrum appears in strong absorption for $R_{\text{in}} \approx 1.3R_\odot$ and weakens toward larger $R_{\text{in}}$. It finally turns to emission for $R_{\text{in}} \approx 1.9R_\odot$. After all, reasonable fits in the 6–7 $\mu$m region, as well as in the near-infrared spectra, can be obtained for $R_{\text{in}} \approx 1.7R_\odot$ (model E) as shown in Figure 9. However, the predicted spectrum shows appreciable excess in the region longward of 7 $\mu$m compared with the ISO spectrum as shown in Figure 9b.

Next, we examine the case of $T_{\text{ex}} = 1750$ K, and reasonable fits in the near-infrared and 6–7 $\mu$m regions are obtained for $R_{\text{in}} \approx 1.5R_\odot$ (model F) as shown in Figures 10a and 10b, respectively. This case is close to the Verhoelst et al. (2006) model except for the column density. We examined their value of $N_{\text{col}} = 2 \times 10^{19}$ cm$^{-2}$, and the resulting near-IR spectrum is shown by the dotted line in Figure 10a. This column density may be too small to explain the H$_2$O 1.4 and 1.9 $\mu$m bands. The peak at 6.6 $\mu$m due to the H$_2$O $\nu_2$ bands can be reasonably accounted for, but the
disagreement in the region longward of 7 μm cannot be resolved as shown in Figure 10b.

For the case of $T_{\text{ex}} = 2000$ K, possible best fits are obtained for $R_{\text{in}} \approx 1.4 R_*$ (model G) as shown in Figure 11. This case is close to the Ohnaka (2004) model except for the column density, and we examined his value of $N_{\text{col}} = 2 \times 10^{20}$ cm$^{-2}$. The resulting near-IR spectrum is shown by the dotted line in Figure 11a, suggesting by Verhoelst et al. (2006). The near-infrared spectrum is relatively insensitive to $T_{\text{ex}}$ and $R_{\text{in}}$ but depends critically on $N_{\text{col}}$. The predicted excess in the region longward of 7 μm compared with the ISO spectrum is somewhat relaxed, but the excess still remains as shown in Figure 11b.

With a hope to improve the fits further, we examined the case of $T_{\text{ex}} = 2250$ K. In this case, $R_{\text{in}} \approx 1.3 R_*$ (model H) results in reasonable fits as shown in Figure 12. Although the fits do not show any drastic improvements, inspection of the cases of $T_{\text{ex}}$ from 1500 to 2250 K reveals that the fits in some details (e.g., strengths of the absorption features, overall shape of the spectra) are generally better for the higher $T_{\text{ex}}$, as can be seen in Figures 9–12. If we further increase $T_{\text{ex}}$ to 2500 K, however, absorption and emission in the 6–7 μm region just cancel for $R_{\text{in}} \approx 1.3 R_*$. Thus, we may stop our survey here, and we summarize the major parameters of the four models discussed above in Table 4.

For α Orionis, the visibility data at the narrow bands as for μ Cephei are not yet known, but those at the broadband K filter are available (Perrin et al. 2004a). We evaluate the band-averaged visibilities for the standard K-band filter as for the narrowband filters discussed in § 3, and we assume that the angular diameter of the central stellar disk is $\theta_0 = 42$ mas following Perrin et al. (2004a). First, we compare the visibility curve predicted for the model photosphere of $T_{\text{ex}} = 3600$ K ($\theta_0 = 10^{-6}$) with the observed visibility data at the K band in Figure 13 and find that it does not fit well to the observed data ($\chi^2 = 300.99$). The case for the extended photosphere ($\theta_0 = 10^{-14}$) discussed in § 2.2 shows only minor changes, and the extended and classical photospheres cannot explain the observed visibilities at the K band.

Next, we compare in Figure 13 the predicted visibilities at the K band for the four models (models E–H in Table 4) discussed above, and the χ² values are 134.26, 102.21, 29.56, and 16.18.
for models E, F, G, and H, respectively. The fits in the first lobe of the visibility curves are better for the models with the higher $T_{\text{ex}}$ and smaller $R_{\text{in}}$ (i.e., model G and especially model H in Table 4). However, the fits in the second and third lobes appear to be more consistent with the models of the lower $T_{\text{ex}}$ and larger $R_{\text{in}}$ (i.e., models E and F in Table 4). The first lobe may reﬂect the basic structure of the object, while the second and third lobes may depend on some ﬁne structures. Thus, considering the consistent results from the infrared spectra and visibilities, we may conclude that the MOLsphere of Betelgeuse is characterized by the rather compact size ($R_{\text{in}} \approx 1.3 R_{\odot}$), rather high temperature ($T_{\text{ex}} \approx 2250$ K), and modest column density ($N_{\text{col}} \approx 10^{20}$ cm$^{-2}$) (i.e., model H of Table 4). Anyhow, it is clear that the visibility data can be interpreted more consistently with the MOLsphere around the photosphere. We conclude that a MOLsphere explains not only the infrared spectra (the mid-IR spectra are discussed in § 4.3) but also the $K$-band visibility data consistently.

4.3. What Do the Mid-Infrared Data Tell Us?

The region shortward of $7.5 \mu m$ discussed in § 4.2 may be almost free from the effect of dust, which, however, will have a signiﬁcant effect on the longer wavelength region. First, we examine the SiO feature near $8 \mu m$, which was used as a further check of the molecular layers by Verhoelst et al. (2006). The band head region of the SiO fundamentals observed by ISO can be reasonably ﬁtted by our prediction with $N_{\text{col}} = 10^{20}$ cm$^{-2}$ as shown in Figure 14, and this column density may not be high enough to mask the photospheric spectrum. However, the ﬁt longward of $7.6 \mu m$ is quite poor, and the ISO spectrum shows a large depression centered at about $8 \mu m$ compared with our prediction. This depression may partly be due to the effect of SiO in the MOLsphere, which we have not considered yet. For simplicity, we have considered only CO and H$_2$O in the MOLsphere, but the effect of other molecules including SiO should certainly be examined. The effect of dust should still be minor in Figure 14, except for a possible tail of the alumina emission suggested by Verhoelst et al. (2006) longward of $8 \mu m$.

In the $10 \mu m$ region, some interesting observations on both spectra and visibilities have been made recently. The interferometric observation in the $11 \mu m$ region revealed that the resulting apparent diameter of $\alpha$ Ori is about 30% larger than those measured in the near-infrared (Weiner et al. 2003). This observation has been made in narrow wavelength bands that are apparently free from molecular lines, and high-resolution spectra conﬁrmed that there is no signiﬁcant spectral feature in the bands. Weiner et al. (2003) interpreted that this result should be due to the effect of the continuum opacity and that the possible presence of hot spots may be responsible for the reduction of the near-IR apparent size. On the other hand, Ohnaka (2004) showed that the apparent large size can be interpreted as due to the H$_2$O opacity of the extended envelope, while H$_2$O absorption lines appear to be weakened because of the ﬁlling in by the emission of the extended envelope. In view of the effect of molecular bands in the $K$-band region in $\alpha$ Ori and $\mu$ Cep, this interpretation may be reasonable as far as the H$_2$O layer is concerned. Also, the effect of the silicate dust shell located far from the stellar surface on the spectra and the visibilities has fully been taken into account.

Recently, Ryde et al. (2006) observed the $12 \mu m$ H$_2$O lines with a higher resolution compared to the previous observations by Jennings & Sada (1998) and argued that the lines should be originating in the photosphere rather than in the extra molecular layers. As a support for this, Ryde et al. (2006) showed that the published realizations of MOLspheres cannot reproduce the observed high-resolution spectra in the $12 \mu m$ region but rather predict the $12 \mu m$ H$_2$O lines in emission. But whether the lines appear in emission or in absorption depends on the parameters assumed, and the absorption spectrum also appears as shown by Ohnaka (2004). Further tests, however, can be done by the details of the spectra such as the line proﬁles and relative intensities, which may differ for the optically thin case suggested by
with the emission of the amorphous alumina ($\text{Al}_2\text{O}_3$). Verhoelst fitted well with their optically thin predictions, and this result considered this effect in their extended model of tailed by Ohnaka (2004): Verhoelst et al. (2006) might have considered with this new dust component in addition to the $\text{H}_2\text{O}$ layer. The alumina shell and the $\text{H}_2\text{O}$ layer are located at about the same height above the photosphere according to Verhoelst et al. (2006), and it is quite possible that only a part of $\text{H}_2\text{O}$ in the MOLsphere will form an optically thin layer above the alumina shell, which may act as a continuum background source for $\text{H}_2\text{O}$ to form absorption. Thus, the observed $12\mu\text{m}$ absorption lines may indeed be produced in an optically thin layer as suggested by Ryde et al. (2006), but this does not imply that they are originating in the photosphere.

Summarizing, the water layer itself may have a rather large column density of about $10^{20}$ cm$^{-2}$, as almost uniquely determined from the Stratoscope spectrum, which is also almost free from the effects of dust. But the mid-infrared water lines may be produced in an optically thin layer, which is only a part of the whole water layer. This explains not only the argument of Ryde et al. (2006) that the mid-infrared water lines are formed in an optically thin layer but also the rather small $\text{H}_2\text{O}$ column density of $2 \times 10^{19}$ cm$^{-2}$ determined from the $11\mu\text{m}$ spectrum by Verhoelst et al. (2006). The column density of $5 \times 10^{18}$ cm$^{-2}$ by Ryde et al. (2006), however, is appreciably smaller than that by Verhoelst et al. (2006). This can be explained by the effect of the emission from the extended part of the molecular layer as detailed by Ohnaka (2004): Verhoelst et al. (2006) might have considered this effect in their extended model of $r \approx 1.4 R$, and then a larger column density is needed to correct for the weakening due to the emission component, while Ryde et al. (2006) assumed photospheric origin without such an effect and then a smaller column density is sufficient just to account for the observed absorption.

As noted by Verhoelst et al. (2006) themselves, however, the presence of the amorphous alumina cloud is still a hypothesis that consistently accounts for the spectral and visibility data, and further confirmation should certainly be required. In recognizing dust in astronomical objects, it is a general difficulty that dust shows no clear spectral signature, but interferometry could recognize the dust cloud with no spectral signature through its geometrical extension. An interesting example is the $N$-band spectrotinterferometric observation of the silicate carbon star IRAS 08002–3803 by Ohnaka et al. (2006), who suggested the presence of a second grain species in addition to silicate around this silicate carbon star. Thus, further detailed interferometry in the mid-infrared region will be quite useful to clarify the nature of the dust species around Betelgeuse. Also, the suggested temperature of 1900 K is too high for $\text{Al}_2\text{O}_3$ to condense in thermal equilibrium at low densities, and some nonequilibrium processes may be required. It is to be noted that even the formation of $\text{H}_2\text{O}$ has the same difficulty of how it is possible to form water in the rarefied outer atmosphere.

In conclusion, by virtue of the alumina dust shell recently suggested on the $\text{ISO}$ spectra by Verhoelst et al. (2006), we found a possibility that all of the mid-infrared observations including the spectra and visibilities can be interpreted consistently at last, but this is possible only if we assume the presence of the extra components, consisting not only of the molecular layer but also of the dust shell beyond the photosphere. Our present model consisting of gaseous molecules alone is certainly not applicable to the mid-infrared region, and, for this reason, we confine our analysis to the region below 7.5 $\mu\text{m}$ where it is almost free of the effects of dust. The next step should certainly be to include warm dust such as alumina as an important ingredient in the outer atmosphere, and we hope that more observations and theoretical analyses for this purpose could be developed.

5. DISCUSSION
5.1. Modelings

Given a model, any observable such as spectrum and visibility can be calculated directly, but the reverse problem to specify a model uniquely from the observed data is not necessarily so straightforward in general. This is because an observed result generally depends on several model parameters. We could determine a set of parameters that are consistent with the known observed data, but this is by no means a unique solution and may be regarded as a possible solution at best. It is to be remembered that even the definitions of the parameters are different by the different authors.

In fact, the definitions of the parameter that specifies the size of the MOLsphere are different. For example, a thin-shell model with no geometrical thickness is characterized by a single parameter: the radius of the thin shell (e.g., Perrin et al. 2005). If the molecular layer extends from the stellar surface to a certain height, a single parameter that specifies the outer radius is sufficient (e.g., Ohnaka 2004). The shell model of a finite thickness requires the inner and outer radii (e.g., Verhoelst et al. 2006). Our models emphasize the inner radius, where the density is the largest, reflecting the starting model photosphere in hydrostatic equilibrium. Nevertheless, the outer radius $R_{out}$ may have some effect, but we have not examined such an effect in detail in this paper. However, we think that it is not useful to increase the number of parameters that may not be very essential.

Detailed parameter fittings may not be our final purpose, but it may be of some interest to know if the molecular layer is very thin or rather thick, or if it is detached or not from the photosphere. Such information can be of some help in considering the origin of the molecular layer, but it may be difficult to decide such details of the geometrical configurations from the interferometric observations at present. However, combined with the spectroscopic data, some information can be obtained. One interesting possibility for this purpose is the case that the gaseous molecules and dust cloud coexist as in the case of water and alumina clouds suggested by Verhoelst et al. (2006). In such a case, the column densities of water estimated from the spectral regions with and without dust background may give a clue for the extent of the water layer (see § 4.3).

As already discussed in § 3.3, it was not possible to have good fits to the observed visibilities at all of the spatial frequencies, and this fact implies that our present modeling is too simplified. Also, our modeling is still a kind of parameter fitting for this simplified model and not a physical modeling yet. Thus, we can have a rough idea on the outer atmosphere of red supergiant

8 For example, if $R_{out}$ is decreased in model C for $\mu$ Cep, then $R_{in}$ must be increased a bit and/or $T_{ex}$ must be changed slightly, to maintain the fits in the visibilities and in the 6.6 $\mu\text{m}$ emission. Thus, many solutions can be possible around a solution such as model C. At present, however, there may be no means by which to discriminate such minor differences in these different solutions.
stars, but this is the present limitation in our modelings. Certainly, our modelings of the available data are to find some clues for a more physical modeling, but it is only recently that the visibility data are made available and we are just starting toward such a purpose. Certainly, more interferometry data for a wider coverage in spectral region and in spacial frequency are highly important.

We assumed the presence of a rather warm gaseous cloud above the photosphere, and the resulting model of the MOLsphere may be rather massive. For example, the H$_2$O column density of $3 \times 10^{20}$ cm$^{-2}$ estimated for $\mu$ Cep may imply a hydrogen column density of the order of $10^{24}$ cm$^{-2}$ if the oxygen abundance in Table 1 can be assumed, and the total mass of the MOLsphere of $\mu$ Cep is as large as $10^{-4} M_\odot$. This will be sufficient as a reservoir for the gaseous mass-loss outflow of about $10^{-7} M_\odot$ yr$^{-1}$ (Josselin et al. 2000). Also, the hydrogen envelope can be large enough for the radio continuum to be opaque, and such an effect is already observed in the radio domain of Betelgeuse (Lim et al. 1998).

Now a more serious problem is how such a new molecular layer can be formed and how it can be stable in the outer atmosphere. We propose it as an observational requirement, and physical interpretation had to be deferred to future studies. However, outer atmospheres of red supergiant and giant stars are not yet well understood, and it is no wonder that such a new feature had to be introduced. In fact, more or less similar features are already known: for example, it has been well accepted that the high-temperature gaseous envelope referred to as the chromosphere exists in the outer atmosphere of cool stars. However, how the chromosphere is formed and how the gaseous matter is transferred to the higher layers above the photosphere have not been known for a long time. In fact, it is possible that the MOLsphere has a close connection to the chromosphere and that they may simply represent cooler and hotter phases of the same phenomenon. From this point of view, a possible outer atmospheric origin of water detected in the K giant star Arcturus by Ryde et al. (2002) may not necessarily be excluded, since the chromosphere is known in this K giant star. Also, in cooler supergiant stars known as maser sources, the presence of huge water clouds is known as an observational fact (§ 5.3). Thus, we think that it useful to accept the presence of the MOLsphere and to investigate its nature with all of the available observational and theoretical possibilities.

Finally, we must also remember that even the photosphere of red supergiants includes many unsolved problems. For example, some infrared lines of OH in Betelgeuse show anomalous intensities that cannot be explained by the photospheric models (e.g., Lambert et al. 1984), and the origin of the supersonic turbulent velocities is also unknown. One interesting problem often mentioned is an inhomogeneity in the photosphere. A possibility of a large inhomogeneity was suggested by Schwarzschild (1975), who argued that only a few convective cells will dominate the stellar surface at one time and produce a temperature inhomogeneity as large as 1000 K. Also, some observations were often interpreted in terms of the inhomogeneity. We have already noticed that the different behaviors of water bands (Ryde et al. 2006) or the measured diameters (Weiner et al. 2003) between the near- and mid-infrared can be due to the photospheric inhomogeneity. Also, imaging of nearby supergiants such as Betelgeuse (e.g., Young et al. 2000) revealed the presence of bright spots on the limb-darkened disk. So far, however, it is not known how these theoretical and observational results can be modeled in a unified picture, and this will be an interesting subject to be investigated further.

5.2. Observations

The observation relatively free from the difficulty noted in § 5.1, namely, that an observed result generally depends on several model parameters, is the near-infrared spectra, which suffer little effect of the extended geometry of the outer atmosphere. As we see in §§ 3 and 4, the column density can be estimated reasonably well from the Stratoscope data alone, and this fact indeed makes the subsequent analysis rather easy. Thus, the Stratoscope data, which were observed 40 years ago, are still unique and invaluable as the probes of the outer atmosphere. Unfortunately, few observations were done in the near-infrared from outside the Earth’s atmosphere since then. However, the near-infrared region can now be observed rather well from the dry sites on the ground, and the near-infrared spectra of higher quality can be obtained without much difficulty. Such observations should be quite useful to examine the accuracies of the data taken nearly half a century ago.

Although the spectra in the region longward of 2.5 $\mu$m were extensively observed especially with the ISO SWS, the H$_2$O 2.7 $\mu$m bands are blended with the other molecular lines such as of CO and OH, while CO and SiO bands include large contributions from the photosphere. For these reasons, the H$_2$O 1.9 $\mu$m bands are the best probes of the outer molecular layers of the early M giant and supergiant stars, and especially the H$_2$O column density can be estimated quite well almost independently of other parameters.

Despite the general difficulty to observe H$_2$O from ground, recent narrowband interferometry by Perrin et al. (2005) demonstrated that the observation of the water layer is possible with the ground-based interferometer and provided decisive evidence for the extra molecular layer in $\mu$ Cep. This is a quite encouraging result in that the ground-based interferometry will already provide fruitful results for the study of the structure of the extra molecular layers in cool luminous stars, before the interferometry in space can be realized.

The H$_2$O $\nu_2$ bands in the 6–7 $\mu$m region are excellent probes of the geometrical extension of the molecular layers but are no longer useful for estimating the column density because they include appreciable emission components from the extended atmospheres and finally turn to emission. Extensive observations of this region were first possible with the ISO SWS. It is interesting to notice that $\mu$ Cep is almost unique in showing the H$_2$O $\nu_2$ bands in emission, except for some Mira variables (Yamamura et al. 1999). Our preliminary survey of dozens of red giant stars in the ISO archive revealed no object with H$_2$O $\nu_2$ bands in emission, although the absorption bands are stronger and weaker in the early and late M giants, respectively, compared with the predictions based on the photospheric models (Tsuji 2002b).

It is to be noted that our modelings of the MOLsphere are done with the use of the spectral and visibility data shortward of 7.5 $\mu$m alone. This has the advantage that the modeling can be done almost independently of the effect of the dust components including the newly identified alumina dust shell (Verhoelst et al. 2006). Also the absorption components still dominate especially in the near-infrared region, and this fact makes the diagnosis relatively easy. In fact, it is almost impossible to determine the column density, if the emission components dominate as in the longer wavelength region. Thus, the basic parameters of the MOLsphere such as $T_{\text{ex}}, N_{\text{col}}$, and $R_{\text{in}}$ are determined from the observations in the shorter wavelength region, while additional information can be obtained from the observations in the longer wavelength region.

The 10 $\mu$m region can be accessible from ground, and detailed interferometry and spectroscopy realized recently for $\alpha$ Ori
provided further constraints and new problems on the outer atmospheres of red supergiant stars, as discussed in § 4.3. It is highly desirable that similar observation of the spectra and visibilities can be extended to the mid-infrared region of \( \mu \) Cep. In the 40 \( \mu m \) region observed with the ISO SWS, water appears in emission in \( \mu \) Cep but only marginally in \( \alpha \) Ori (Tsuji 2000b). Our preliminary version of model A plus the silicate dust shell could reproduce the whole SWS spectrum of \( \mu \) Cep between 2.5 and 45 \( \mu m \) reasonably well (Tsuji 2002b). Thus, our MOLsphere model shows overall consistency with the observed infrared spectrum covering a wide spectral range. However, some details such as the relative intensities of some emission lines do not necessarily agree very well with the predicted thermal emission spectra, and further detailed analysis including the non-LTE effect should be needed.

The bright red supergiant stars have also been targets of extensive radio observations, and one of the highlights may be the VLA mapping of Betelgeuse at 7 mm by Lim et al. (1998), who showed that the temperatures over the same height range as the chromosphere (e.g., from \( \approx 2R_c \) to \( \approx 3R_c \)) are appreciably cooler (correspondingly from 3450 ± 850 to 1370 ± 330 K) than the temperatures generally assumed for the chromosphere (e.g., 8000 K). Our MOLsphere may be situated just inside of such a "radio photosphere," after a naming by Reid & Menten (1997), and covers the region not well resolved with the radio interferometry. A detailed modeling of the outer atmosphere of Betelgeuse based on the radio data has been done by Harper et al. (2001), who also surveyed a large number of observations covering from UV to centimeter regions. It seems that inhomogeneity must be considered for all of the multiwavelength data to be integrated into a unified picture of the outer atmosphere of red supergiant stars. This fact also suggests that the interrelation between the molosphere and the stellar chromosphere should be investigated more carefully.

### 5.3. Water in Red Supergiant Stars

Within the limitation of the present modeling discussed above, the extra molecular layers of \( \alpha \) Orionis and \( \mu \) Cephei seem to show interesting differences. The MOLsphere of \( \alpha \) Orionis is relatively hot (\( T_{ex} \approx 2250 \) K) and compact (\( R_{mol} \approx 1.3R_c \)), while that of \( \mu \) Cephei is cooler (\( T_{ex} \approx 1600 \) K) and more extended (\( R_{mol} \approx 2.0R_c \)). It is interesting if such a change may represent an evolution of the outer atmosphere in the supergiant evolution.

probably a more advanced stage of the evolution of the outer atmosphere in red supergiants may be represented by such objects as VY CMa and S Per. In these objects, infrared excess is very large, indicating that the dust envelope should be very thick. The gaseous components in the outer atmosphere are more difficult to observe and, even though these supergiants were extensively observed with ISO (e.g., Tsuji et al. 1997b; Harwit et al. 2001), little is known yet. On the other hand, these red supergiants are known as the maser sources. Of particular interest is that water appears to be quite abundant in the outer space of these red supergiants. Recent VLBI observations revealed that water forms masering clouds around VY CMa (Imai et al. 1997) and S Per (Richards et al. 1999).

The origin of the masering water clouds may not be known yet. It is an interesting possibility that the MOLsphere in the early M supergiants will develop to the masering water clouds in the later M supergiants. But the origin of the MOLsphere itself is unknown. It may also be possible that an unknown water supply will provide water to the MOLsphere, as well as to the masering clouds. Anyhow some mechanism is needed to enhance the matter density in the outer atmosphere around red supergiants stars, either transporting more matter from the central star or else accreting some matter from the outer space. Certainly we are still far from realizing the recycling of water around evolved stars, and comparative studies of objects in the different stages of developing the outer atmosphere will be useful for this purpose.

### 6. CONCLUDING REMARKS

The presence of the extra molecular layers in the outer atmosphere of red supergiant stars has been anticipated from the infrared spectra for the first time. With the spectra alone, however, it was difficult to exclude a possibility that the unexpected spectral features may be due to anomalous structures of the stellar photospheres. Recent interferometric observations in different spectral regions finally provided decisive evidence for the presence of the extra molecular layers outside the stellar photosphere.

On the other hand, interpretation of the visibility data alone may be by no means unique since the present interferometric observations do not yet reconstruct the astronomical image directly. For this reason, simultaneous analysis of the spectral and visibility data should be quite essential. Certainly, multiwavelength interferometry such as done recently by Perrin et al. (2005) already includes some spectroscopic information in itself, and future spatial interferometry with a higher spectral resolution will hopefully involve all of the necessary spectroscopic information.

Thanks to the fine achievements, in both the spectroscopy and interferometry, we are convinced of the presence of the extra molecular layers outside the stellar photosphere. Now, an important problem is how to understand the presence of such a rather warm and dense molecular layer outside the photosphere. This problem may be related to that of the stellar chromosphere, for which detailed modelings have been done but its origin may be by no means clear yet. Probably, the problem of the origin of the MOLsphere may be as difficult as that of the chromosphere and will require comprehensive understanding of the whole outer atmosphere. We hope that more attention, both observational and theoretical, could be directed to this problem of the extra molecular layer, or the MOLsphere, in view of the convincing confirmation of its existence in the outer atmospheres of red supergiant stars.

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INFRARED SPECTRA AND VISIBILITIES

Note added in proof.—Our hope expressed in \S 5.2 that the mid-infrared spectra of $\mu$ Cephei could be observed has just been realized in a recent work by Ryde, N., Richter, M. J., Harper, G.M., Eriksson, K., & Lambert D. L. (ApJ, press [2006], astro-ph/0603384). The result is quite unexpected in that the pure rotation lines of water in the 12 $\mu$m region appeared in definite absorption. As shown by the authors themselves, their result cannot easily be fitted to a MOLsphere model, which predicts the 12 $\mu$m water lines in emission. This result is quite difficult to understand, since we know from the $ISO$ data of $\mu$ Cep that water lines appear in emission not only in the 6 $\mu$m but also in the 40 $\mu$m regions, and these results could have been explained by our MOLsphere model. Therefore, the 12 $\mu$m water absorption may be a local phenomenon in this region, which may suffer the largest effect of dust opacities. We have already discussed a complication, possibly due to the warm alumina grains in the mid-infrared region of $\alpha$ Orionis, in \S 4.3, and a more or less similar consideration may be applied to $\mu$ Cep. We have also assumed that our MOLsphere model is isothermal but this should most probably be an oversimplification. If the MOLsphere has a thermal structure something like the stellar protosphere, normally cooler in the outer part, then the absorption lines can be formed in the MOLsphere itself under the presence of the continuum opacity sources possibly due to dust. (Here, a problem is how dust could be accommodated in the outer atmosphere under the possible effect of the radiation pressure.) The water absorption lines observed in the mid-infrared region reveal the extreme complexities of the outer atmosphere of red supergiants stars and offer a strong new constraint on its structure. We should like to remind the reader that our models discussed in this paper are consistent with the observed data shortward of 7.5 $\mu$m, which are almost free from the effect of dust, and hopefully represent the basic features of the gaseous molecular layers in the outer atmosphere.