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LETTER

Letter to the Editor

Line formation in the Atmosphere of brown dwarf Gliese 229B : CH_4 at 2.3 μ m

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Abstract. We investigate the formation of methane line at 2.3 $\mu\mathrm{m}$ in Brown Dwarf Gliese 229B. Two sets of model parameters with (a) $T_{\mathrm{eff}} = 940\,\mathrm{K}$ and $\log(g) = 5.0$, (b) $T_{\mathrm{eff}} = 1030\,\mathrm{K}$ and $\log(g) = 5.5$ are adopted both of which provide excellent fit for the synthetic continuum spectra with the observed flux at a wide range of wavelengths. In the absence of observational data for individual molecular lines, we set the additional parameters that are needed in order to model the individual lines by fitting the calculated flux with the observed flux at the continuum. A significant difference in the amount of flux at the core of the line is found with the two different models although the flux at the continuum remains the same. Hence, we show that if spectroscopic observation at $2.3\mu\mathrm{m}$ with a resolution as high as $R \simeq 200,000$ is possible then a much better constraint on the surface gravity and on the metallicity of the object could be obtained by fitting the theoretical model of individual molecular line with the observed data.

Key words: molecular processes – line: formation – radiative transfer – stars: low-mass, brown dwarfs

1. Introduction

The discovery of methane bands in the spectrum of Gl 229B (Nakajima et al. 1995, Oppenheimer, Kulkarni, Matthews & Nakajima 1995, Geballe, Kulkarni, Woodward, & Sloan 1996) has not only helped to identify Gl 229B as a Brown Dwarf but also prompted the creation of the new spectral class of T dwarfs (Kirkpatrick et al. 1999). The synthetic continuum spectra of the object has been obtained with and without dust particles (Marley et al. 1996, Griffith, Yelle & Marley 1998, for a review see Allard et al. 1997). Although the incorporation of condensates can explain the very rapid decline of the observed continuum flux in the optical region, it is shown (Tsuji, Ohnaka, & Aoki 1999, Burrows, Marley, & Sharp 1999) that the pressure broadened red wing of the 0.77 $\mu\mathrm{m}$ K I doublet could also account for the observed features of the continuum flux shortward of 1.1 $\mu\mathrm{m}$. The spectrum of the first field methane T dwarf SDSS 1624+0029 shows a broad band absorption feature centered at 7700 Å which is interpreted (Liebert et al. 2000) as the K I 7665/7699 resonance doublet. Hence, it is most likely that the shape of the red spectrum is due to the broad wings of the K I and the Na I doublets and not due to the presence of condensates. All these model spectra together with the bolometric luminosity of the object (Leggett et al. 1999) and the evolutionary sequences (Saumon et al. 1996) can constrain the effective temperature of the object very tightly, however the surface gravity is still poorly constrained. It is shown (Saumon et al. 2000) that a multi-parameter fit of the observed spectrum both for the K-band and for the red end is possible with different metallicities. Therefore, in order to determine the physical properties of the atmosphere of Gl 229B and the other T dwarfs uniquely, more comprehensive theoretical modeling of the observed spectrum is required. One of the most important studies is the individual line formation by the most abundant molecules, eg. CH_4, H_2O, NH_3 etc.

In this paper, we for the first time, attempt to model the line formed by methane at 2.3 $\mu\mathrm{m}$ and show that if individual lines of abundant molecules, in particular that of methane can be resolved observationally, then stringent constraint on the surface gravity, on the metallicity and on the temperature at the bottom of the atmosphere, where the optical depth is very high, can be obtained.

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2. The line transfer equations

In order to model the individual line of a particular molecule one needs to solve the Non-LTE line transfer equations. The two level atom line transfer equation in the plane parallel stratified medium can be written as (Mihalas 1978)

$$\pm\,\mu\frac{\partial I(\nu,\pm\mu,z)}{\partial z} = k(\nu,z)[S(\nu,\pm\mu,z) - I(\nu,\pm\mu,z)]\,, \quad (1)$$

where μ is the cosine of the angle made by the ray to the normal. The total absorption coefficient $k(\nu,z) = k_l(z)\phi(\nu,z) + k_c(\nu,z)$, where k_l is the frequency integrated line absorption coefficient, $\beta(z) = k_c/k_l$, k_c is the absorption coefficient for the continuum and $\phi(\nu, z)$ is the line profile function. The source function is given by

$$S(\nu, \pm\mu, z) = \frac{\phi(\nu, z)S_l(\nu, \pm\mu, z) + \beta(z)S_c(z)}{\phi(\nu, z) + \beta(z)}, \quad (2)$$

where S_c is the continuum source function which is set equal to the Planck function $B(\nu, z)$ and the line source function S_l is written as

$$S_l(\nu, \pm\mu, z) = \frac{1-\epsilon}{2} \int_0^\infty \phi(\nu', z) d\nu' \times$$
$$\int_{-1}^{1} R(\nu, \mu : \nu', \mu') I(\nu', \mu', z) d\mu' + \epsilon B(\nu, z)\,, \quad (3)$$

where ϵ is the probability per scattering that the photon is destroyed by collisional de-excitation and is given by (Mihalas 1978) $\epsilon \equiv \epsilon'/(1+\epsilon')$; $\epsilon' \equiv C_{ul}(1-e^{h\nu/kT})/A_{ul}$, C_{ul} is the rate of collisional de-excitation and A_{ul} is the rate of spontaneous emission. R is the redistribution function defined according to a hybrid model prescription by Rees & Saliba (1982) and is given by $R(\nu, \mu; \nu', \mu') = P(\mu, \mu')R(\nu, \nu')$, where $P(\mu, \mu')$ is the phase function and $R(\nu, \nu')$ is the angle-averaged frequency redistribution function for isotropic scattering.

3. The absorption coefficient

Under chemical equilibrium among different atomic and molecular species in their standard states, the number density of CH_4 for the molecular equilibrium reaction $C + 2H_2 \rightleftharpoons CH_4$ can be written as (Sharp 1985)

$$n_{CH_4} = n_C n_{H_2}^2 \left(\frac{h^2}{2\pi mkT}\right)^3 10^{D_o\Theta} \frac{Q_{CH_4}}{Q_C Q_{H_2}^2}, \quad (4)$$

where Q_C and Q_{H_2} are the partition functions for C and H_2, m is the "multiple" reduced mass and D_o is the dissociation energy of CH_4 in eV, n_C and n_{H_2} are the number densities of C and H_2, $\Theta(z) = 5040/T(z)$ where $T(z)$ is in Kelvin, and the other symbols have their usual meaning. Although chemical equilibrium of C and H_2 should be coupled with some other molecules, dominance of CH_4 molecule in the atmosphere would make the above equilibrium the most probable one. Hence, we ignore, for the present, chemical equilibrium of C and H_2 with other molecules. For the purpose of calculating the number densities of the molecules in various energy levels, we assume that the lower atmosphere of the object is in local thermodynamic equilibrium (LTE). Then the number of particles n_J, in a specified rotation level J is related to the total number of particles in all levels, n_{CH_4}, according to the following relation (Larson 1994):

$$\frac{n_J}{n_{CH_4}} = \frac{(2J+1)e^{-E_J/kT(z)}}{Q_{CH_4}}, \quad (5)$$

where (2J+1) is the degeneracy factor and $e^{-E_J/kT}$ is the Boltzmann factor. Now the integrated line absorption coefficient can be written as

$$k_l(z) = \frac{\pi e^2}{m_e c} f n_J(z) = \frac{\pi e^2}{m_e c} f \left[\frac{h^2}{2\pi mkT(z)}\right]^3 10^{D_o\Theta(z)} \times$$
$$\frac{(2J+1)e^{-E_J/kT(z)}}{Q_C Q_{H_2}^2} n_C(z) n_{H_2}^2(z)\,, \quad (6)$$

where f is the oscillator strength of the transition. We calculate the Q's for H_2 and C using polynomial expressions given by Sauval & Tatum(1984). For a small value of J, the Boltzmann factor reduces to 1. The dissociation energy D_o of CH_4 is taken to be 4.38 eV (Jorgenson 1994). We use the continuum absorption coefficient k_c provided by D. Saumon.

4. The synthetic continuum spectra in the infrared region

We present the synthetic continuum spectra of Gl 229B (Fig. 1) in the infra-red region where the signature of methane is clear and dominant. The monochromatic radiative transfer equations are solved numerically by using discrete space theory (Peraiah and Grant 1973). We have adopted two sets of model parameters, model (a): $T_{\rm eff}$=940 K, log g=5.0 (g in cm s^{-2}) and [M/H]=-0.3 (K band) and model (b): $T_{\rm eff}$=1030 K, log g=5.5 and [M/H]=-0.1 (K band). The temperature and pressure profiles for both the models are obtained from M. Marley (private communication). The values of $T_{\rm eff}$ and the surface gravity g are constrained by the bolometric luminosity of Gl 229B and the evolutionary sequence of Saumon et al. (1996). These synthetic spectra fit the entire observed spectrum of Gl 229B except in the near infra-red region. It should be mentioned that a good fit with the observational data for the entire wavelength region is not possible with the same value of the metallicity and the surface gravity. The above sets of model parameters are two of many optimal sets of parameters that can produce good fit. In order to match the observed flux shortward of 1.1 μm that declines very rapidly, either dust particulates or alkali metals have to be incorporated. However, the size of the grain that is needed to explain the observed spectrum in the optical region is too small to play any role in the infra-red region we are interested in the present work. Hence in this spectral region the law of Mie scattering that describes the angular distribution of photons in a dusty atmosphere reduces to that of Rayleigh scattering. Therefore, the synthetic spectrum in this region matches well with the observed flux when Rayleigh's law of scattering is used. Recent ovservational evidence (Liebert et al. 2000) implies that there is no compelling reason to introduce dust or additional opacity source in the atmosphere of methane dwarf. Therefore in the present work we have not incorporated dust opacity.

Fig. 1 shows that there is no difference in the calculated continuum flux with the two sets of model parameters. Both the models fit the observed data very well.

5. Results and discussion

The continuum opacity and the temperature-pressure profile of the atmosphere are set by matching the synthetic continuum spectrum with the observed spectrum for the entire wavelength region. The modeling of individual lines needs the values of additional parameters. In the absence of observational data for individual lines, we set the value of these parameters by matching the calculated flux in the continuum with the observed con-

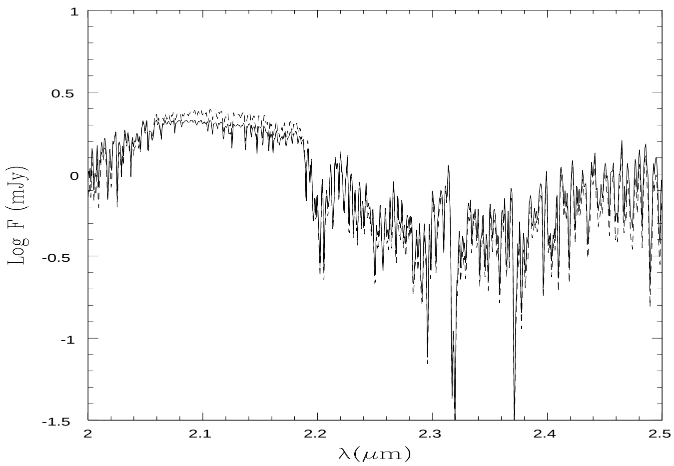

Fig. 1. Synthetic continuum spectrum of Gl 229B: broken line is for the model (a) with $T_{\rm eff} = 940\,{\rm K}$ and $log(g) = 5.0$ (g in ${\rm cm\,s^{-2}}$), solid line for the model (b) with $T_{\rm eff} = 1030\,{\rm K}$ and $log(g) = 5.5$

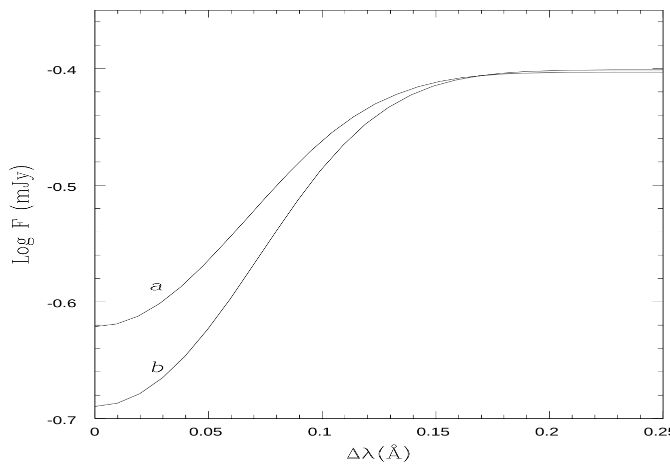

Fig. 2. Emergent flux against wavelength from the line center ($2.3\mu{\rm m}$): the curve 'a' is for the model (a) and the curve 'b' is for the model (b)

tinuum flux at 2.3 μm. Since the line is very weak in intensity, we choose the profile function as (Mihalas 1978)

$$\phi(\nu, z) = \frac{1}{\sqrt{\pi}\Delta\nu_D(z)} e^{-[(\nu-\nu_0)/\Delta\nu_D(z)]^2}, \qquad (7)$$

where $\Delta\nu_D$ is the thermal Doppler width and ν_0 is the line center. It should be worth mentioning that individual molecular lines are usually not saturated enough so that pressure broadening is less important for them as compared to strong atomic lines. Moreover, molecular lines often overlap so strongly that their wings are completely masked (Schweitzer et al. 1996) and only the Gaussian line cores of the strongest molecular transitions are observed. The atmosphere of a brown dwarf is therefore only weakly sensitive to the Van der Walls damping constant. Nothing is known, at present, about the rotation of the brown dwarf Gl 229B around its own axis of rotation. If the projected velocity '$v \sin i$' of the object is greater than 2 to $5\,{\rm km s^{-1}}$ then rotational broadening could be significant. However, in the present work we have neglected rotational broadening in order to make the results consistent with the calculation of the evolutionary sequences by Saumon et al. (1996) that constrains the surface gravity and the effective temperature of the object. The whole purpose of the present work is to show that with different values of the surface gravity and the metallicity, the flux at the line core is significantly different although it is the same in the continuum. Since rotational broadening would affect the spectrum equally for both the models, it is not important in the context of the present work. We assume complete frequency redistribution and use Rayleigh phase function for the angular redistribution.

The parameters that are to be set in order to model the CH_4 line at 2.3 μm are ϵ, f, $n_C(z)$, $n_{H_2}(z)$, and the degeneracy factor $(2J+1)$. We define $s = (2J+1) f n_C(z) n^2_{H_2}(z)$ guided by equation (6) and set the values of s and ϵ such that the calculated value of the flux at the continuum matches with the observed continuum flux. We assume that ϵ is independent of the geometrical depth. This is valid if the CH_4 line formation is confined to a narrow region in the atmosphere. After testing several empirical laws we adopt the usual inverse square law with respect to the geometrical depth for the variation of the number density of C and H_2. This should be verified when observational data becomes available. Experimental determination of the oscillator strengths for different transitions at 2.3 μm and at the relevant temperature could further constrain the number density of C and H_2 and hence the abundance of methane in the atmosphere of Gl 229B provided chemical equilibrium exists between the molecule and the atoms. We have solved the radiative line transfer equations by using discrete space theory (Peraiah 1980). The theoretical models for the methane line at 2.3 μm are presented in Fig. 2. For the model (a) we find that the flux at the continuum matches with its observed value when $\epsilon = 0.08$ and $s = (2J+1) f n_1 n_2^2 = 5.9 \times 10^{37}$ where n_1 and n_2 are the number densities of C and H_2 respectively at the bottom of the atmosphere. The moderately high value of ϵ is consistent with the temperature at the lower atmosphere where the lines are formed. For the model (b) the flux at the continuum matches with the observed flux when $\epsilon = 0.08$ and $s = 2.7 \times 10^{39}$. Since the temperature of the lower atmosphere for the two models does not differ much, the value of ϵ remains the same for both the models. However s differs substantially for the two models. This is because of the fact that for the model (a) the continuum opacity is less and therefore one has to reduce the line opacity in order to keep the right ratio (β) between them so that the calculated flux matches with the observed flux at the continuum. However, the higher value of s in the model (b) makes the line opacity higher than that for the model (a) and so substantial decrease in the calculated flux at the line core is obtained. The difference in the flux reduces as we go towards the wings. It is worth mentioning that the wings could be masked by other lines whereas the continuum is overlapped by several lines.

Fig. 2 shows that a spectral resolution as high as 200,000 at $2.3\mu{\rm m}$ is needed in order to investigate the individual molecular lines. This may be possible with an appropriate combination of the telescope and the instrument. For example, the Cooled Grating Spectrometer 4 (CGS4) available in UKIRT

(United Kingdome Infra-Red Telescope) has a spectral resolution upto 40,000. If observation of Gl 229B is possible at present by UKIRT with the maximum resolution power of CGS4 then keeping the signal to noise ratio (which is proportional to the diameter of the telescope and to the square root of the integration time of exposure) unaltered, a 10 m telescope (such as Keck I) can obtain the desired resolution by using a similar type of spectrometer provided the resolution of the instrument is increased by about five times and the integration time of exposure is increased by about 2.5 times.

It is found that the numerical values of ϵ and s are very much sensitive to the emergent flux. The difference in the flux at the line core is clearly due to the different values of the surface gravity and the metallicity. Theoretical modeling of the continuum flux provides a few possible combinations of the metallicity, surface gravity and the effective temperature that are appropriate in explaining the observed continuum flux. The observational fit of the flux at the line core would decide which one of these combinations should describe the physical properties of the atmosphere. The physical parameters that are needed to model the individual molecular line will also be fixed once observational data is available. Therefore, in conclusion we would like to emphasize that a theoretical fitting of the observed flux for the individual lines of any of the dominant molecules, especially methane, would not only provide a much better understanding on the abundance of that molecule and the temperature of the lower atmosphere but also improve the constraints on the value of the surface gravity of brown dwarfs.

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