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Chemical equilibrium and spectra of ultracool dwarfs

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Abstract. Some problems of computations of the chemical equilibrium in the atmospheres of ultracool dwarfs are discussed. Computations in the framework of the classical approach provide the wrong fluxes in the spectra of dwarfs of the effective temperature $T_{\rm eff} \leq 3000$ K. In fact we had to use for them the semiempirical model atmospheres to fit our synthetic spectra to the observed ones. Our results of computations of the chemical equilibrium in atmospheres of Y-dwarfs and the planetary mass objects are presented.

Key words. Stars: abundances – Stars: atmospheres – Stars: Population II – Galaxy: globular clusters – Galaxy: abundances – Cosmology: observations

1. Introduction

Before 1995 only a few individual observations of the peculiar spectra of low-mass objects were known (see Kirkpatrick et al. 1993). For the past 18 years the picture of our understanding of the population of objects at the bottom of the Hertzsprung-Russell has changed drastically. In 1995 the discoveries of first brown dwarfs and planetary mass objects (exoplanets) were reported (see Rebolo et al. 1995; Nakajima et al. 1995; Mayor & Queloz 1995). They were followed by an avalanche-like growth in the number of low mass objects, resulting in the implementation of the new spectral classes L and T (see Martín et al. 1997, 1999; Kirkpatrick et al. 1999). Substantial progress in discovering dwarfs of these spectral types was achieved during last decades by The Sloan Digital Sky Survey (SDSS) and the Two Micron All Sky Survey (2MASS) and other promising surveys (see contributions of of María Rosa Zapatero Osorio, Víctor Béjar, Adam Burgasser, and others in this volume). Moreover, first reports about discovery of the cooler dwarfs of spectral classes Y with effective temperatures of 300 - 800 K appeared recently (Cushing et al. 2011). Generally speaking, we understand the nature and physics of these very cool and very faint objects. The cooler T dwarfs are bluer in colors in comparison with L-dwarfs (Kirkpatrick et al. 1999; Burgasser et al. 1999, 2000). However, we can claim to understand the processes in atmospheres of L-dwarfs only if we can model the reliable spectra and colors of ultracool dwarfs. Unfortunately, the unified theory of the formation of ultracool dwarfs of spectral classes L, T, and Y has been under construction until now (see the talk of France Allard in this volume). In this paper we investigate the chem-

Send offprint requests to: Ya. Pavlenko istry of some molecular and atomic species which are the important opacity sources that govern the optical and infrared spectra of ultracool dwarfs. We draw special attention to the chemical equilibrium of potassium and sodium in the atmospheres of ultracool dwarfs. The extended wings of such absorption lines govern the near infrared part of the spectrum of L and T dwarfs (see Pavlenko 1997, 1998).

2. Procedure

Chemical equilibrium in the atmospheres of ultracool dwarfs was computed in the framework of the Local Thermodynamic Equilibrium (LTE) for the mix of ≈100 molecular species. Alkali-contained species formation processes were considered in detail because of the important role of the neutral alkali atoms in the formation of the spectra. Constants for chemical equilibrium computations from Gurvitz et al. (1982) were converted to the Kurucz (1970) format. In the Kurucz's ATLAS programs a computationally convenient format is used:

$$\frac{\prod_i^l N_i}{N_{1,2,...l}} = \exp[-E_{1,2,...l}/kT + g(T)],$$

where the function $g(T)$ is given by:

$$g(T) = b - c(T + d(T - e(T + fT))) + \frac{3}{2}(l - p - 1)\ln T \qquad (1)$$

In our work the values of b, c, d, e are determined by the fitting to the Gurvitz et al. (1982) data using the least square minimisation procedure for the temperature range 100 - 5000 K.

3. Results

3.1. H contained species

Molecular densities of some important species in the atmospheres of dwarfs of $T_{\rm eff}$= 1600, 1200, 800, 500 K are shown in Fig. 1. The dependence of the computed molecular densities on the temperature is clearly seen. Similar dependences were studied by different authors see (see Tsuji 1973), however, in our case the temperatures in the outer parts of photospheres are lower, i.e. they are of order a few hundreds K. In the comparatively "hot" atmosphere of $T_{\rm eff}$= 1600 K molecular density depends, in the first approach, on the dissociation potential of the molecules. We find interesting the case of the atmosphere of $T_{\rm eff}$= 500 K. In the outer part the molecular densities of CH_4 and NH_3 are larger than N_2. Still H_2 densities dominate over the whole atmosphere. Left top panel of Fig. 2 shows the densities of the hydrogen contained species in atmosphere of the 500/4.0/0.0 dwarf. Ions H^+ are not shown there due to their low densities. We see the clear drop of densities oh H atoms toward the outer boundary of atmosphere. In the atmospheres of hotter solar-like stars density of H atoms increases toward outer layer of the stellar photosphere. In this case most atoms of H are captured by other molecular species and, as a result, density of H atom is lower than density of He atom over most of the atmosphere. This has at least three important implications:

a) To compute the pressure broadening of atomic (and molecular) lines even in the outer part of atmospheres, we should account interactions with H_2, He, H_2O and N_2 (see top right panel of Fig. 1).
b) Our computations show that densities of ions of metals with lower than H potential of ionisation and electron densities, in the outer part of the atmosphere are very low.
c) Physical conditions on the low boundary of ultracool atmosphere are very hard to be modelled properly. Broadening of lines and physical state of the astrophysical plasma at 10-100 atm may differ drastically from the known case of hotter stars.

All of these factors turn off H^- opacity, and, consequently, increase the importance of the processes of scattering on the molecules H_2, H_2O, and the atoms He.

3.2. Na and K

As it was noted above, the extended wings of Na I and K I resonance lines govern the spectral energy distributions in the optical and near

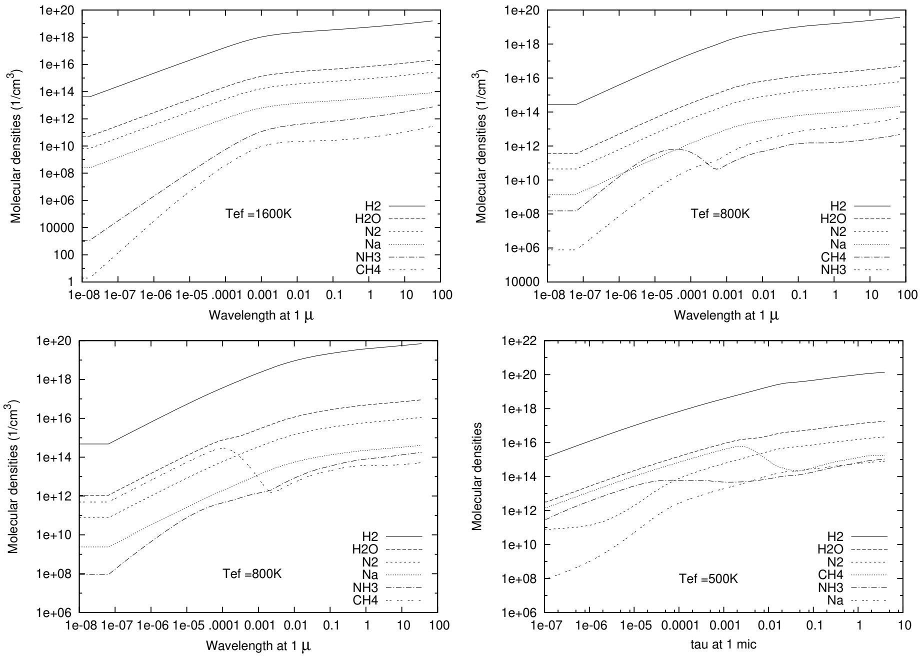

Fig. 1. Molecular densities of some species which are the important sources of opacity in the atmospheres of ultracool dwarfs computed for the DUSTY model atmospheres of $T_{\rm eff}$= 1600, 1200, 800, 500 K and solar metallicity from Allard et al. (2001).

infrared spectral regions of ultracool dwarfs of spectral classes L and later. Formation of some molecules containing K and Na atoms would, in principle, reduce the number of these atoms in the atmospheres of the ultracool dwarfs and, respectively, reduce the intensity of K I and Na I resonance lines in their spectra. To study the problem, we recomputed the dissociation constants of molecules contained atoms Na I and K I for the case of temperatures $100 < T < 5000$ K. Molecular equilibrium was computed for the model atmosphere 500/4.0/0 from the Allard et al. (2001) grid. Results for Na and K are shown in Fig. 2. Indeed, K and Na atoms are bound into molecules NaOH and KOH, and n(NaOH) > n(Na) and n(KOH) > n(K) at least in the outer part of photospheres of ultracool dwarfs. However, our direct computations show that the effects of depletion of K and Na atoms into molecules cannot reduce the huge strengths of their resonance lines in the spectra of dwarfs of $T_{\rm eff}$< 800 K.

4. Discussion

Our results were obtained in the framework of the classical approach, i.e. we assumed the Local Thermodynamic Equilibrium (LTE), plane parallel atmosphere without sinks and sources of energy. We do not consider any dynamical processes. Then, we do not account for the dust formation processes. On the other hand, our computations show that the most of the atoms of metals are bound into different molecules. Nevertheless, atoms of elements can be depleted by the dust particle formation processes. In that sense our results show the upper limit of formation of molecules.

Our results show that the substantial part of potassium and sodium atoms are bound in NaOH and KOH molecules, especially in the outer parts of ultracool atmospheres. However, these processes cannot reduce the densities of K and Na atoms even in the atmospheres of ultracool dwarfs of $T_{\rm eff}$< 800 K.

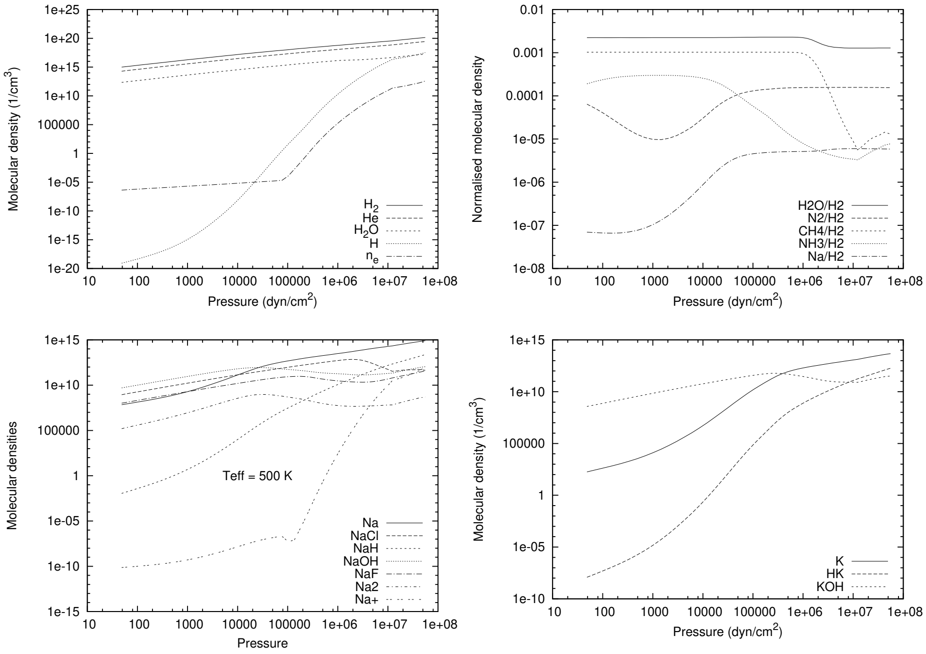

Fig. 2. Molecular densities of some important species in atmosphere of ultracool dwarf of $T_{\rm eff} = 500$ K, $\log g = 5.0$ and solar metallicity. Top panels shows the most abundant molecular species contained hydrogen atom (left), and relative molecular densities $n_i/n_{(H_2)}$ (right). Bottom panel shows the densities of molecules contained sodium (left) and potassium (right) atoms.

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