

Formation of lithium lines in very cool dwarfs

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Received 1 September 1994 / Accepted 4 April 1995

Abstract. We present LTE and NLTE results on the formation of Li I lines ($\lambda 6103$, $\lambda 6708$, and $\lambda 8126$) in the atmospheres of solar metallicity dwarfs with effective temperatures in the range 5500 K to 2000 K. NLTE effects are governed by overionization of Li and by the interlocking effects of energy levels. For stars with $T_{\text{eff}} \geq 4000$ K, we confirm previous findings by Magazzù et al. (1992). NLTE corrections can lower the LTE Li abundances derived from strong Li I $\lambda 6708$ lines by up to 0.5 dex.

Our computations using model atmospheres with T_{eff} between 3000 K and 2000 K show that prominent Li I lines are formed. We give a set of line profiles, which support the feasibility of the Li test for brown dwarfs. The ionization-dissociation equilibrium for Li species was carefully considered. NLTE effects on the Li I lines of very cool dwarfs are found to be small, implying corrections to the LTE Li abundances lower than 0.1 dex. Several numerical tests have been carried out to estimate the effects of chromosphere-like structures on the formation of Li I lines. Our preliminary results suggest that in the presence of very strong chromospheres, the line strengths are reduced.

Key words: line: formation – stars: late type; brown dwarfs – stars: abundances

1. Introduction

The most numerous stars in the solar neighbourhood are the low mass dwarfs. Studies of these stars are relevant to the understanding of many important issues in modern astrophysics, including stellar evolution, nucleosynthesis and stellar atmospheres. The atmospheres of G-K dwarfs can be compared with the Sun, but the coolest dwarfs are more complicated.

Spectroscopic studies are hampered by many problems that remain to be solved: refinement of basic stellar parameters (T_{eff} , $\log g$, microturbulence, metallicity); improvement of atmospheric modelling; more accurate molecular data; incorpo-

ration of a large number of opacity sources; and the effects of the departure from LTE.

In the last few years several works have contributed to alleviate these problems. For instance, computations of very cool atmospheres have become available (e.g., Allard 1990). Our aim is to use these model atmospheres to study the formation of spectral lines of astrophysical interest, to interpret high resolution spectra, and in particular to derive photospheric chemical abundances.

In this paper we analyze the formation of Li I lines in the atmospheres of solar metallicity late-type stars (T_{eff} : 2000–5000 K). In former papers (Magazzù et al. 1992; Martín et al. 1992, 1994a; García López et al. 1994) we have presented results of LTE and NLTE calculations of the Li I resonance doublet in dwarfs with $T_{\text{eff}} \geq 3500$ K (G, K and early M-type stars). Here, we present a few new results on these stars and an extension to much lower effective temperatures. The computations for $T_{\text{eff}} \leq 3000$ K are relevant to the search for brown dwarfs (BDs). A spectroscopic test able to directly confirm the substellar nature of BD candidates has been recently put forward (Rebolo et al. 1992). It consists in the detection of the Li I $\lambda 6708$ feature, due to the fact that Li rapidly disappears from the atmospheres of very low mass stars, but it is preserved in BDs with masses less than about $0.065 M_{\odot}$ (Magazzù, Martín & Rebolo 1993, see also Bessell & Stringfellow 1993 for a review). High resolution spectroscopic observations have so far failed to detect Li in a number of BD candidates (Magazzù et al. 1993; Marcy et al. 1994; Martín et al. 1994b), thereby constraining their masses to be larger than $0.065 M_{\odot}$. The computations of Li I lines in very cool dwarfs will help to plan future Li searches in BD candidates, and they provide a theoretical framework for interpreting future Li detections in substellar objects.

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2. The procedure

2.1. The spectral synthesis code: WITA2

The spectra of dwarfs with $T_{\text{eff}} \lesssim 4000$ K are formed by blends of a huge number of molecular and atomic lines. To compute synthetic spectra we used the WITA2 program, which is a part of the ABEL6 complex (Pavlenko 1991), composed partly from Kurucz (1979) ATLAS's subprograms. The WITA2 computations were performed in the frame of the classical approach: LTE and hydrostatic equilibrium for one-dimensional model atmospheres. This code allows to extrapolate the model atmosphere and/or build a simple model chromosphere using two parameters: T_{min} and G_{rad} - minimum and temperature gradient, respectively. The ionization-dissociation equilibria equations system has been solved for various temperature structures assuming local thermodynamical equilibrium. A Voigt profile was adopted for single absorption lines. The algorithm of damping constant computations will be considered in detail in Sect. 2.5.

2.2. Opacities, atomic and molecular data

In the state equation system we considered 21 atoms in two ionization states and 54 molecules. In particular, we have considered seven molecules containing Li. In Table 1 we give the molecular data used to compute the dissociation equilibrium of this element. The data for all the molecular species were taken from Tsuji (1973). Opacities due to continuum absorption of radiation were computed by Kurucz's ATLAS subprograms.

In our computations we also used two sets of opacity sources:

- i. For $T_{\text{eff}} > 4500$ K we only took into account opacities due to absorption by atomic lines from Kurucz (1992).
- ii. For $T_{\text{eff}} \leq 4500$ K the opacities due to molecular lines absorption were included as well.

Molecular features are dominant in the spectra of M-stars. Unfortunately the lack of good and complete line lists of numerous molecules makes difficult the numerical analysis of the spectra of very cool stars. In this work we used two approaches to describe the absorption features due to molecular bands.

- i. In the region around the Li I $\lambda 6708$ doublet we used the "line by line" computation. The molecular line list was the same as used by Abia et al. (1993) in their study of Li in carbon red giants, and it includes lines of TiO, ^{12}CN and ^{13}CN . We changed the oscillator strengths of some lines around the Li I $\lambda 6708$ doublet to match the observed spectrum of the M-dwarf UX Tau C (see Sect. 3.2).

- ii. We also used the Just Overlapping Approximation (JOLA approach) following Yaremchuk's approach (see Nersisyan et al. 1987). Allard (1990) and Kirkpatrick et al. (1993) used a similar approach in their spectral synthesis computations. Yaremchuk's approach has the advantage of taking into account the split to P-Q-R branches of each molecular band. The computations were performed for vibrational quantum numbers in the range $0 < v', v'' < 9$. We have verified that our computations of the TiO bands in the region of the LiI resonance doublet

correctly describe the positions and intensities of the observed bands in very cool M-dwarf spectra.

The constants of electronic and vibrational transitions were taken from Huber & Herzberg (1979), Kuznezova et al. (1980), and Kuz'menko et al. (1984). The molecular band systems data used in the JOLA approximations are given in Table 2. These molecular data were used to synthesize the spectra of the coolest stars considered in this paper and in the NLTE computations to obtain the radiation field fluxes in the frequencies of the Li I bound-free transitions.

2.3. Model atmospheres

We used model atmospheres from two grids, computed under the classical assumptions. For $T_{\text{eff}} \geq 3500$ K we have used the grid of models produced by Kurucz (1992), computed using the new Kurucz molecular and atomic line opacities using the Opacity Sampling (OS) method. For T_{eff} between 3000 K and 2000 K we used the grid of models by Allard (1990). They were computed using the JOLA approximation to treat molecular band absorption. All the models here were computed for solar abundances and microturbulent velocities of 2 km s^{-1} . When this work was in preparation, new M-dwarf model atmospheres became available (Allard et al. 1994). We have confirmed that the use of these new models do not change the main conclusions of our work.

In order to get a correct solution of the radiative transfer equation, we extrapolated these model atmospheres up to a level where monochromatic optical depths in the center of the Li I resonance doublet are less than 0.01, as in the paper by Magazzù et al. (1992).

2.4. Non-LTE procedure

To solve the NLTE problem for the Li I atom we used the Auer & Heasley (1976) complete linearization method. In detail our approach was described in Pavlenko (1989) and Magazzù et al. (1992). Here we use a Li I atom model of 20-levels (see for details Pavlenko 1994). Atomic level data were taken from Wiese et al. (1966). We checked that the main qualitative results were already obtained using a model of only 6-levels. In our computations 70 radiative and all possible collisional transitions due to free electrons and neutral hydrogen were included into the rate matrix. The cross-sections for the radiative and inelastic collisional transitions were adopted from the same references given in Magazzù et al. (1992). We caution that there is not final conclusion on the reliability of the approaches describing the rates of inelastic collisions due to neutral hydrogen (e.g. Lambert 1993). We performed additional computations to investigate the impact of these rates on our results. We found that for M-dwarf atmospheres the influence of inelastic collisions with neutral hydrogen is not critical because hydrogen is mainly in molecular form, and the statistical balance of lithium is governed by radiative processes.

The ten strongest radiative bound-bound transitions from the ground and first excited level of Li I $\lambda 6708$ were linearized and

Table 1. Lithium molecular data

Molecule	D0	b	c	d	e	f
LiH	2.429	4.4990E+01	2.2310E-03	4.6440E-07	4.7180E-11	1.7730E-15
LiO	3.514	4.6220E+01	2.2560E-03	4.7700E-07	4.8840E-11	1.8440E-15
LiF	5.943	4.6720E+01	2.2090E-03	4.5440E-07	4.6130E-11	1.7370E-15
LiCl	4.902	4.5950E+01	2.2390E-03	4.5730E-07	4.6420E-11	1.7520E-15
LiBr	4.381	4.6020E+01	2.3360E-03	4.8970E-07	5.0260E-11	1.9080E-15
LiI	3.687	4.6020E+01	2.5090E-03	5.3250E-07	5.4930E-11	2.0920E-15
LiOH	8.893	2.7250E+02	1.1930E-01	2.9690E-05	3.2460E-09	1.2820E-13

Molecular constants of Li molecules included in the NMOLEC program used in this work (see for details Kurucz, 1970).

Table 2. Molecular data

N	Molecule	System	Transition	f_e	Q_{ij}	$\lambda_1-\lambda_2$
1	VO		$B^4\Pi \Rightarrow X^4\Sigma^-$	0.04 (A90)	A90	7400 – 9300
2	VO	A-X		0.0026 (A90)	A90	9460 – 12800
3	TiO	Φ	$b^1\Pi \rightarrow d^1\Sigma^+$	0.02 (B89)	K84	7900 – 18000
4	TiO	γ'	$B^3\Pi \Rightarrow X^3\Delta$	0.08 (B89)	K84	4800 – 8500
5	TiO	γ	$A^3\Phi \Rightarrow X^3\Delta$	0.09 (B89)	K84	5400 – 10550
6	TiO	ϵ		0.0024 (B89)	K84	7500 – 9470
7	TiO	δ	$b^1\Pi \Rightarrow a^1\Delta$	0.02 (B89)	K84	6450 – 12800
8	TiO	β	$c^1\Phi \Rightarrow a^1\Delta$	0.15 (B89)	K84	4800 – 7000
9	TiO	α	$C^3\Delta \Rightarrow X^3\Delta$	0.10 (B89)	K84	3900 – 7750
10	SO		$A^3\Pi \Rightarrow X^3\Sigma^-$	0.21 (K80)	K84	2460 – 3800
11	SiO		$D^1\Pi \Rightarrow X^1\Sigma^+$	0.16 (K80)	K84	2070 – 3300
12	NO	$\pi 3p \delta$ bands	$C^2\Pi_r \Rightarrow X^2\Pi$	0.015 (K80)	K84	2070 – 2750
13	NO	β bands	$B^2\Pi_r \Rightarrow X^2\Pi$	0.0035 (K80)	K84	2000 – 3800
14	NO	$\sigma 3s \gamma$ bands	$A^2\Sigma^+ \Rightarrow X^2\Pi_r$	0.0020 (K80)	K84	1950 – 3400
15	MgO		$B^1\Sigma^+ \rightarrow X^1\Sigma^+$	0.048 (K80)	K84	4540 – 5440
16	MgH		$A^2\Pi_r \Rightarrow X^2\Sigma^+$	0.059 (K80)	K84	4100 – 6400
17	CO		$A^1\Pi \Rightarrow X^1\Sigma^+$	0.12 (K80)	K84	1140 – 2800
18	CN		$A^2\Pi_i \Rightarrow X^2\Sigma^+$	0.0011 (K80)	K84	4000 – 56300
19	CN		$B^2\Sigma^+ \Rightarrow X^2\Sigma^+$	0.036 (K80)	K84	2400 – 6000
20	BO		$A^2\Pi \Rightarrow X^2\Sigma^+$	0.035 (K80)	K84	2900 – 5700
21	AlO		$B^2\Sigma^+ \Rightarrow X^2\Sigma^+$	0.039 (K80)	K84	4040 – 5800

Note: f_e are electronic oscillator strengths and their source, Q_{ij} are Franck-Condon factors and sources, $\lambda_1-\lambda_2$ are the wavelength ranges where the molecular bands are significant.

References: (A90) Allard 1990, (B89) Brett 1989, (K80) Kuznezova et al. 1980, (K84) Kuz'menko et al. 1984.

the line multiple structure was considered in detail (Pavlenko 1989). For the $\lambda 6708$ transition we took into account “line by line” absorptions due both to atomic and TiO and CN lines. In the rest of the linearized transitions only atomic absorptions were included. Most of the linearised lines lay in the blue and UV part of the spectrum where atomic absorption is extremely strong and the addition of new opacity sources should not change significantly the NLTE results. For stars with $T_{\text{eff}} \geq 4500$ K the role of these molecular absorptions is very small and our results are correct. Neglecting them at lower effective temperatures imply that we will obtain an upper limit to the NLTE effects. The other radiative bound-bound transitions were included into computations with “fixed radiative rates”. We adopt $J_\nu^l = J_\nu^c$, where J_ν^c is the mean intensity of the radiative field in the continuum

and J_ν^l in the line. At the frequencies of “fixed rates” radiative bound-free Li I transitions we adopted

$$\kappa_{\text{tot}} = \kappa_c + \kappa_l + \kappa_{\text{JOLA}} \quad (1)$$

where κ_{tot} , κ_c , κ_l , κ_{JOLA} are the total opacity, and opacities due to continuum, lines, and JOLA molecular bands absorption, respectively (we assume $\kappa_l = 0$ for $\lambda > 8000$ Å). To compute the radiation field in the frequencies of bound-free transitions we averaged the radiation field mean intensity (see Pavlenko 1991; Magazzú et al. 1992). We note that the NLTE ionization equilibrium of Li is mainly governed by the radiation field in the frequencies of the transition 2-continuum (Pavlenko 1991).

Using the JOLA method we have investigated the effects of ultraviolet molecular absorptions on the radiation field at the frequencies of bound-free transitions of Li I. Although it

would be preferable to use a detailed “line by line” computation, in the case of strong molecular absorptions it is expected that our approximation produces a good result. Molecular absorptions produce a significant effect even at $T_{\text{eff}} = 4500$ K. We note that our molecular absorption band list is far from being complete, and hence it is expected the real effects to be larger. At $T_{\text{eff}} = 5000$ K and hotter, these effects become smaller.

2.5. Damping constants of Li I lines

In the coolest stellar atmospheres with high lithium abundance the Li I resonance lines become saturated. Due to the high pressure in the atmospheres of cool dwarfs ($\log g \sim 5$), van der Waals damping is strong and the resonance Li I lines show extended wings. In our previous works (e.g. Magazzù et al. 1992) we used for damping constant computation the equation given in Kurucz (1979):

$$C_6 = \text{const} * (N(H) + N(He) * 0.42 + N(H_2) * 0.85) \quad (2)$$

where *const* is a constant determined by Unsold (1955) approximation, and $N(H)$, $N(He)$, $N(H_2)$ are densities of neutral H and He atoms, and H_2 molecules, respectively. In the present computation we have applied a multiplicative factor E to C_6 . For most iron lines this factor lies in the range $1 < E < 2$ (cf., Kostik 1991). In our case, its determination is an important issue, since the strength of the Li I lines will be strongly dependent on it, particularly for the higher abundances. Li I and Na I have similar atom term structures, so we expect that damping affects their line wings in similar way. Theoretical 6-8-12 interatomic potential computations of Andretta et al. (1981) give for the resonance Li I D_2 line and Na I D_1 lines $E=1.50$ and 1.62 , respectively. It is remarkable that these values, obtained for solar-like model atmospheres, are similar for both resonance lines. We made some numerical experiments to test the reliability of our damping constant computations. At first we reproduced the Na I D_1 lines in the solar spectrum observed by Kurucz et al. (1984). WITA2 computations were performed for the HOLMU model atmosphere (Holweger & Müller 1974), Kurucz (1992) line list (modified in some cases) and microturbulence velocity $v_t=1 \text{ km s}^{-1}$. A comparison with the solar observed spectrum showed that the best result was obtained for $E=2$ (Fig. 1). Our result is slightly different to the one obtained by Andretta et al. (1981), as expected from the use of a different expression for C_6 in which the dependence on quantum number l was ignored.

In the solar atmosphere, we have $N(H_2) \ll N(H)$, so it's not possible to make a conclusion on the role of the H_2 molecule in van der Waals damping. Such role increases towards lower effective temperatures. In the spectrum of cool dwarfs the resonance Na I lines are severely blended by molecular bands, but there are two subordinate Na I lines in the red, lying in a comparatively weak blended region around 8200 Å (e.g., Kirkpatrick et al. 1991), which can be used to refine our damping constant determination. We tried to reproduce those lines in the spectrum of a very cool dwarf observed by Martín et al. (1994b), namely LHS 2065, spectral class M9V, and adopted for our analysis the Allard (1990) model atmosphere ($T_{\text{eff}} = 2500$, $\log$

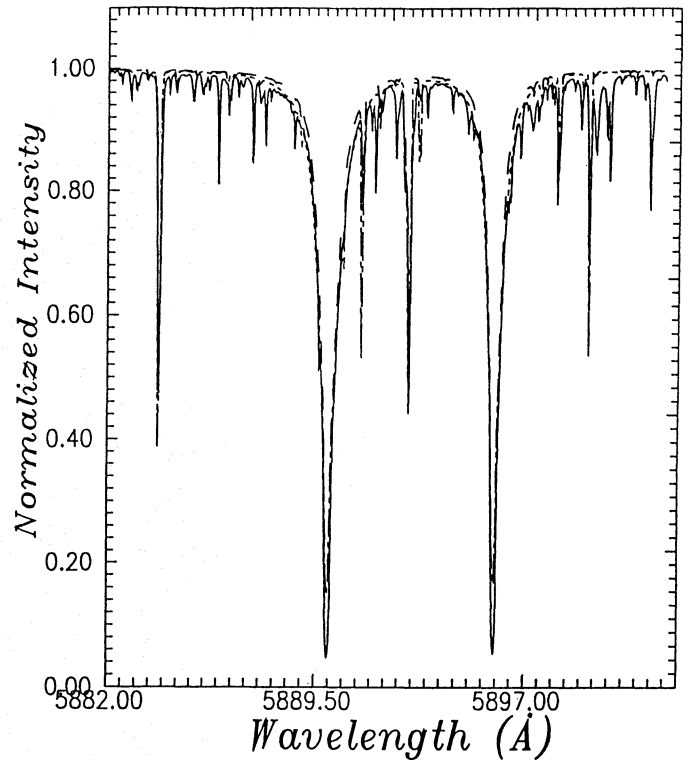


Fig. 1. Spectral synthesis fits to the Na I D_1 lines in the solar spectrum of Kurucz et al. (1984). We show the effects of considering damping due to H_2 molecules and H atoms (short dashed line), and only H atoms (long dashed line). In both cases we used $E=2$. The solid line shows the observed solar spectrum

$g=5.0$, solar metallicity) closest to the stellar parameters estimated by Martín et al. (1994b). We used a microturbulence velocity $v_t = 2 \text{ km s}^{-1}$. The list of atomic lines was taken from Kurucz (1992) and molecular opacities were computed in JOLA approximation. All the molecular bands from Table 2 that lie in that spectral region were taken into account. Our aim was to fit the central intensity and half-width of the Na I lines. The core of the strong Na I lines may be affected by NLTE. However, most of Na atoms in the atmosphere of such a cool dwarf must exist in neutral form and, in principle, the NLTE effects for this element should not be large. We produced LTE synthetic spectra, which were convolved with a gaussian of a width adequate to reproduce the spectral resolution of the observation. The results of our computations are shown in Fig. 2. We found that:

- Equation 2 overestimates the effect of van der Waals damping due to molecular H_2 .
- the best match to the observed spectrum is obtained when only damping due to neutral hydrogen and helium atoms is considered and E takes a value of 2. Hence, in the following work we have adopted for damping

$$A = E \times \text{const} \times (N(H) + 0.42 \times N(He)) \quad , \quad E = 2.0(3)$$

This damping constant has to be taken with caution since we have not carried out an extensive investigation of the role of molecular hydrogen collisional rates (which we feel is out

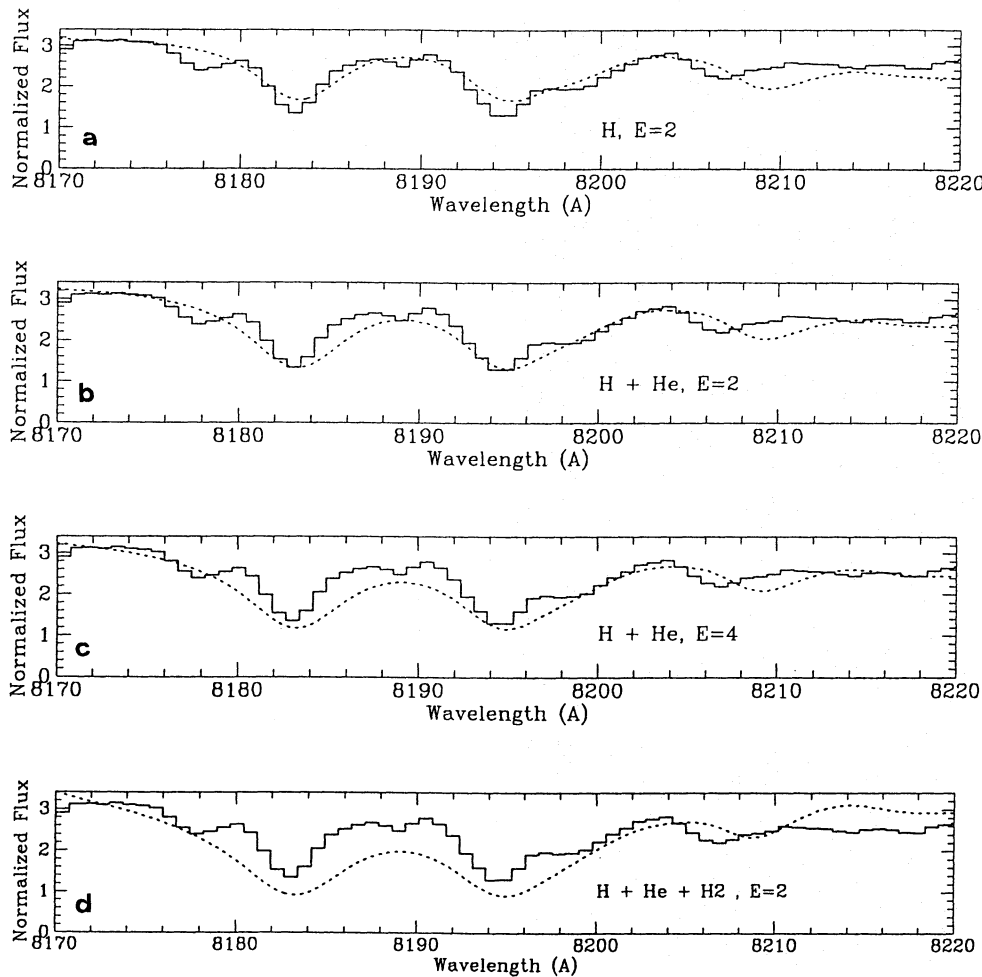


Fig. 2a–d. Spectral synthesis fits (dotted lines) to the Na I $\lambda\lambda 8183, 8195$ lines in the spectrum (solid lines) of the M9 dwarf LHS 2065 of Martín et al. (1994b). From top to bottom we show computations using damping due to: **a** only H atoms ($E=2$), **b** H and He atoms ($E=2$), **c** H and He atoms ($E=4$), **d** H and He atoms, and H_2 molecules ($E=2$)

of the scope of this paper). Dismissing the molecular hydrogen term appears necessary, but the possibility remains that the neutral hydrogen damping term is inaccurate and H_2 has to be considered.

2.6. Formation of Li molecules

Using the molecular data given in Table 1 we investigated the dependence of the ratio $n(\text{Li I})/n_t(\text{Li})$ on optical depth where $n(\text{Li I})$ is the number density of neutral Li atoms, $n_t(\text{Li})$ is the total number density of Li contained species (neutral atoms, ions and molecules). Our results for several model atmospheres considered in this paper are presented in Fig. 3. We find that in the atmospheres of stars with $T_{\text{eff}} \geq 4000$ K, $n(\text{Li I}) \ll n_t$, i.e. most of the lithium atoms exist in the form of ions. So in these atmospheres the overionization may play an important role because small changes in the ionization equilibria could produce significant changes of $n(\text{Li I})$. Our computations show that the densities of molecules containing Li atoms are small in comparison with $n(\text{Li I}) + n(\text{Li II})$.

On the contrary, in the photospheres of M-dwarfs with $2500 \leq T_{\text{eff}} \leq 3000$ K Li mostly exists in the neutral form. In that case the overionization effects should not play a significant role. At lower T_{eff} most of the Li atoms are bound into molecules in

the outer part of the atmosphere. We have therefore considered the formation of molecular species of Li at T_{eff} below 3000 K for reliable determinations of Li abundances in the atmospheres of such cool objects. We must note that the Li I resonance lines are formed in this case at the background of saturated TiO lines.

3. NLTE results

3.1. Models with T_{eff} in the range 3500–5500 K

We present results obtained with a 20-level Li atom model, with damping constants given by Eq. 3 for $E=2$ and new opacity sources due to molecular absorption, especially important for cool atmospheres at the frequencies of Li I bound-free transitions. This set of computations improves those presented in Magazzù et al. (1992), and have partly been published by Martín et al. (1994a), who applied them to the abundance analysis of Li in weak T Tauri stars.

We computed LTE and NLTE curves of growth for each line linearized in the NLTE computations. Most of these lines lay in the UV part of spectrum severely blended by lines of other elements. In Figs. 4, 5 and 6 we present the LTE and NLTE curves of growth of the Li I lines at $\lambda 6708$, $\lambda 6103$ and $\lambda 8126$, obtained using solar metallicity Kurucz (1992) models

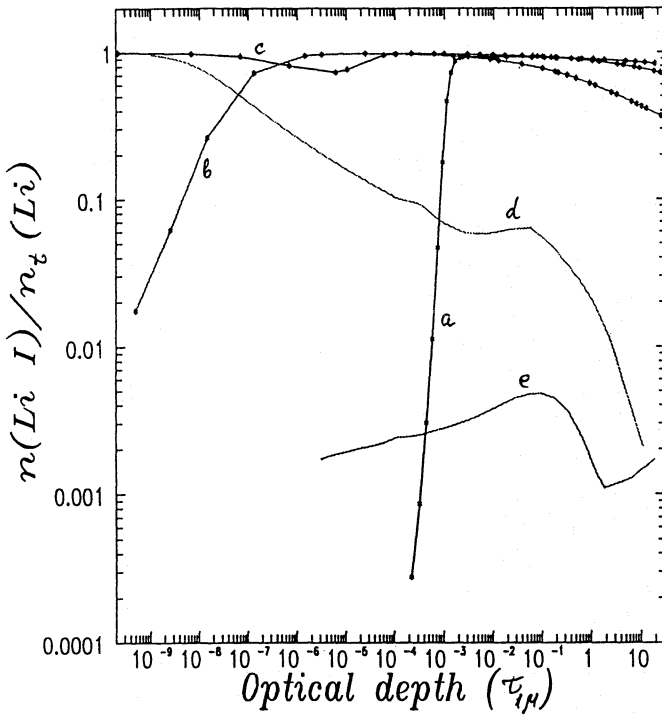


Fig. 3. The ratio $n(\text{Li I}) / n_e(\text{Li})$ versus τ_{μ} computed for the 2000/5.0 (a), 3000/5.0 (b), 2500/5.0 (c), 4000/4.0 (d) and 5000/4.0 (e) model atmospheres

with the following $T_{\text{eff}} / \log g$: 5500/4.5, 4500/4.5, 3500/4.5. We note that:

1) For weak and unsaturated lines ($W \leq 200 \text{ mÅ}$) an over-ionization effect dominates: $W_{\text{LTE}} \geq W_{\text{NLTE}}$. The strength of the NLTE profiles is lower than the LTE profiles both in the core and in the wings (see for an example Fig. 7).

2) When the Li I lines become saturated, we have

$$W_{\text{LTE}} \leq W_{\text{NLTE}}.$$

The cores of the NLTE profiles are stronger (Fig. 7), because in such case $S_{ij}(\tau_{\text{nlte}} = 1) < B_{\nu}(\tau_{\text{lte}} = 1)$ and $r_{\nu}^{\text{nlte}} < r_{\nu}^{\text{lte}}$ (cf. Magazzù et al. 1992).

3) For the subordinate Li I line $\lambda 6103$ we find $W_{\text{LTE}} \geq W_{\text{NLTE}}$ for models in the T_{eff} range 4500 to 5500 K. But for the model of $T_{\text{eff}} = 3500 \text{ K}$ we have $W_{\text{LTE}} \leq W_{\text{NLTE}}$.

4. In general, we have obtained small NLTE corrections for the Li I line at $\lambda 8126$. The sign of the NLTE abundance corrections also change for the lowest T_{eff} model considered (3500 K) $W_{\text{LTE}} \leq W_{\text{NLTE}}$, while for hotter models we find an opposite behaviour.

The main difference between the present results and those in Magazzù et al. (1992), is found for saturated resonance lines in the model with 4000/4.0, where we find opposite sign to the NLTE equivalent width correction. Such discrepancy is due to our use of a more complete model atom. In general, it is expected that when the number of levels in the model atom decreases the interlocking effects are weakened (see Steenbock & Holweger 1984). In addition, Magazzù et al. used an expression for damping constant including broadening of Li I lines by

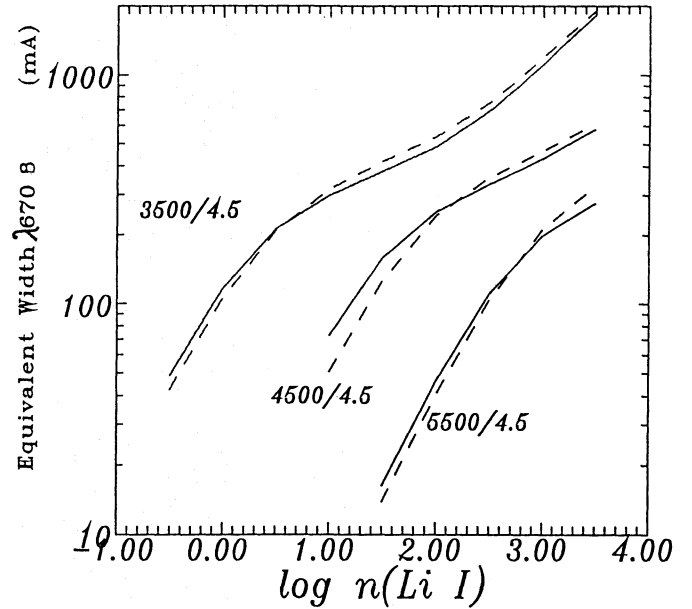


Fig. 4. LTE (solid) and NLTE (dashed) curves of growth for the Li I $\lambda 6708$ line using atmosphere models with 5500/4.5, 4500/4.5, 3500/4.5

molecular hydrogen. Finally, in this work we have taken into consideration additional opacities due to molecular bands.

When this work was in preparation, a paper by Carlsson et al. (1994) was published addressing the NLTE effects on the formation of the Li lines in stellar atmospheres. They used different opacity sources, a different NLTE spectral synthesis code and different model atmospheres. In spite of this, their results confirm previous findings in Magazzù et al. (1992) for high gravity solar metallicity stars and are also in general good agreement with our present computations (see also Pavlenko 1994, 1995).

3.2. The coolest stars

As was noted above the Li I lines in the spectra of stars with $T_{\text{eff}} < 4000 \text{ K}$ (M spectral types) become severely blended by numerous molecular lines. The Li I resonance lines lie in a region where the absorption due to TiO molecular bands is dominant.

We investigated NLTE effects on the formation of Li I lines using the same basic procedure described above. Since Li exists mainly in neutral and molecular form in the atmospheres of very cool dwarfs we do not expect significant NLTE effects. This was confirmed by our direct computations for Allard model atmospheres with T_{eff} in the range 3000 to 2000 K, and $\log g = 5.0$.

In Fig. 8 we present the departure coefficients of lithium levels $b_i = n_i / n_i^*$, in the atmosphere of a dwarf 2500/5.0/0. Here n_i^* and n_i are the NLTE and LTE populations of the lithium levels, respectively. We found: 1) In the outer part of the atmosphere ($\tau_{\mu 1} \leq 10^{-3}$) b_1 and b_2 are less than 1, these levels are underpopulated as compared with LTE. 2) The other levels are overpopulated. They are more bounded to the continuum than to the lowest levels.

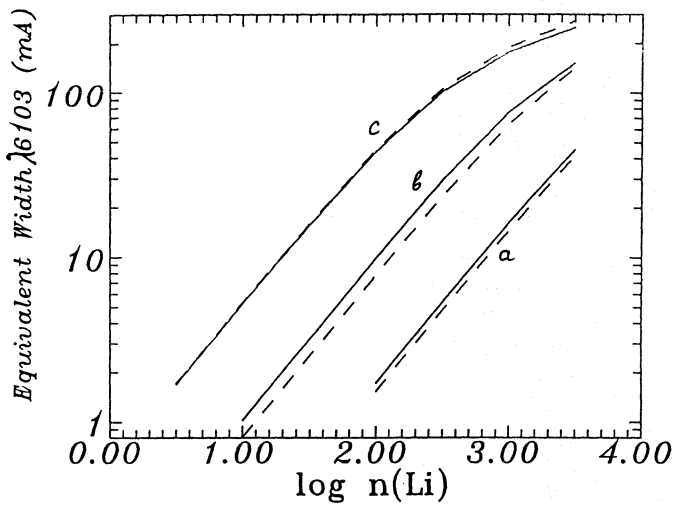


Fig. 5. LTE (solid) and NLTE (dashed) curves of growth for the Li I $\lambda 6103$ using atmosphere models with 5500/4.5 (a), 4500/4.5 (b), 3500/4.5 (c)

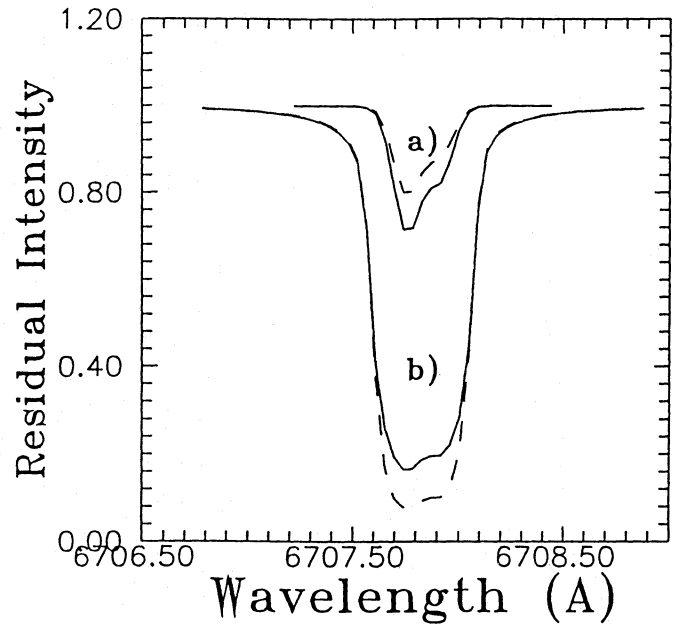


Fig. 7a and b. Theoretical LTE (solid) and NLTE (dashed) profiles of Li I $\lambda 6708$ doublet for model atmosphere with 4500/4.5 and $\log n(\text{Li})=1.0$ (a) and 3.0 (b)

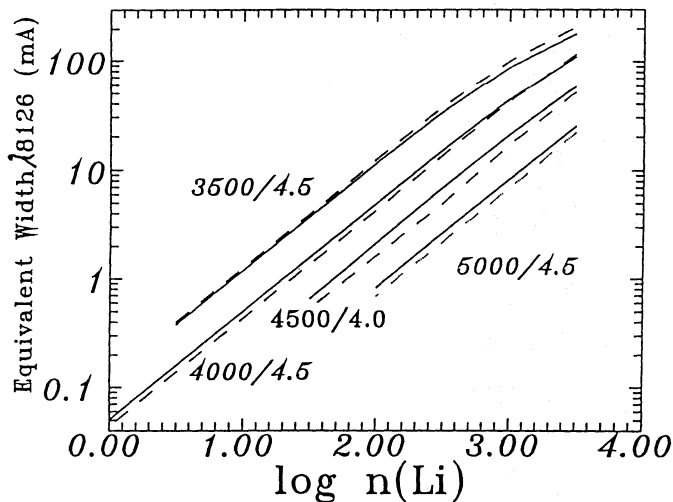


Fig. 6. LTE (solid) and NLTE (dashed) curves of growth for the Li I $\lambda 8126$ line using atmosphere models with 5000/4.5, 4500/4.0, 4000/4.5 and 3500/4.5

We note that the electron density in the dwarf atmosphere 2500/5.0 is extremely low, so the chains of transitions to first and second levels are not so effective as in G-K dwarf atmospheres, where for saturated Li I resonance doublet lines we have found $b_1 > 1.0$, in a wide range of depths (see Pavlenko 1994, 1995; Carlsson et al. 1994). Also, for this cool dwarf we obtained $b_2 > b_1$ and $S_l > B_\nu$ (Fig. 8, 9). The thermalisation of the strong resonance transition occurs at $\tau_{1\mu} = 10^{-5}$. We cannot use the notion “overionization of lithium” in the traditional sense. We may speak, however, about the overpopulation or the under-

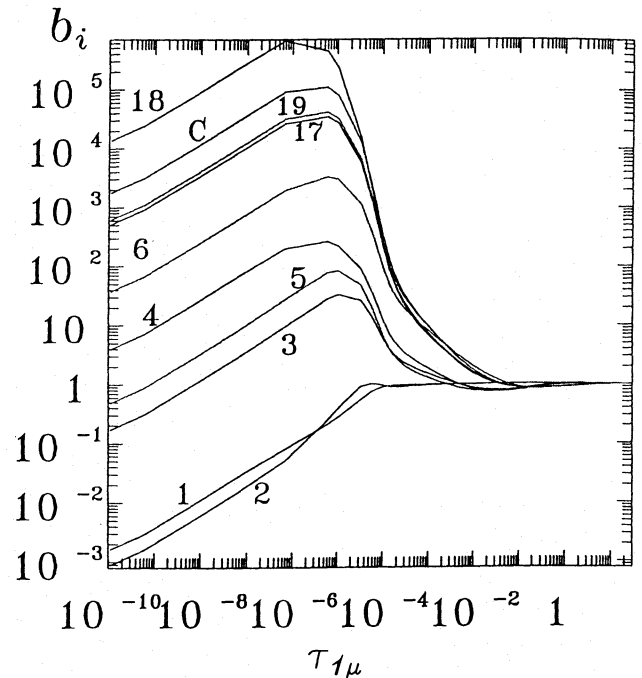


Fig. 8. Departure coefficients of the Li I atoms in a model atmosphere with solar metallicity, $T_{\text{eff}}=2500$ K and $\log g=5.0$. The curves are labelled with the number of the corresponding atomic level. C denotes the continuum level

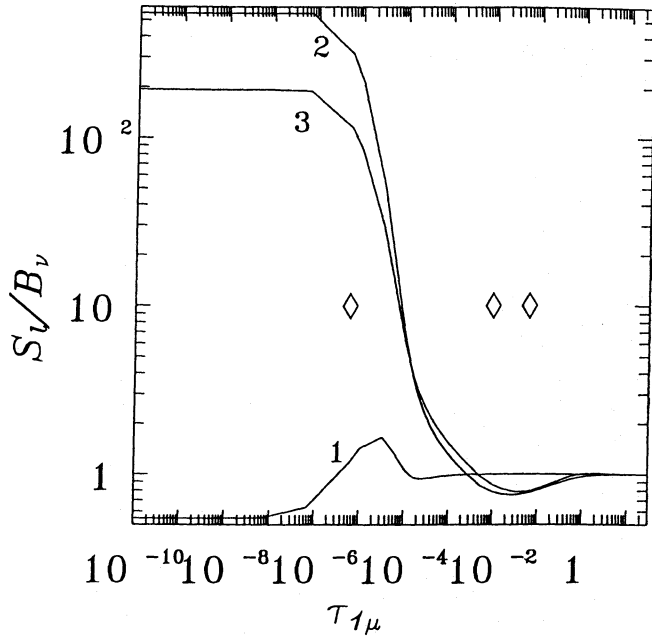


Fig. 9. The ratio between the source and Planck functions S_l/B_ν for Li I lines: (1) - resonance lines 670.8 nm, (2), (3) - subordinate lines 812.6 and 610.3 nm, respectively. Diamonds present the core formation depths of the Li I lines 670.8 nm, 610.3 and 812.6 nm from left to right

populations of lithium levels. The behaviour of the departure coefficient of the third and higher levels depends on the electron temperature and electron density. Up to an optical depth of 10^{-5} the temperature in the model atmosphere decreases, so the populations of lithium levels are controlled by the disbalance of bound-free transitions. In a zero-order approach we may suggest that photoionization processes are controlled by the radiation temperature, and the photorecombination processes are controlled by the electron temperature. In the outer part of the atmosphere the electron temperature T_e drops, while the radiative temperature is constant due to small radiation absorption, hence at small τ the overionization of lithium increases. Above $\tau = 10^{-5}$ the temperature in the model atmosphere is nearly constant, however the departure coefficients of the first and second lithium levels drops here due to the decrease of the electron density.

In conclusion, we found:

i.) NLTE effects for strong lithium lines in the atmospheres of cool M-dwarfs are small. The abundance correction $\Delta \log n(\text{Li}) = \log n_{\text{NLTE}}(\text{Li}) - \log n_{\text{LTE}}(\text{Li})$ is less than 0.1 dex.

ii.) The NLTE abundance correction for the subordinate lines were always negative. The correction for the resonance line was negative in the 2000 K model, and in the 3000 K if $\log n(\text{Li}) \geq 2.0$

Since the NLTE effects were not significant we decided to use LTE computations to produce a set of Li I profiles useful for comparison with observations.

In Figs. 10, 11 and 12 we present some synthetical spectra of M-dwarfs in this spectral region. They were computed using

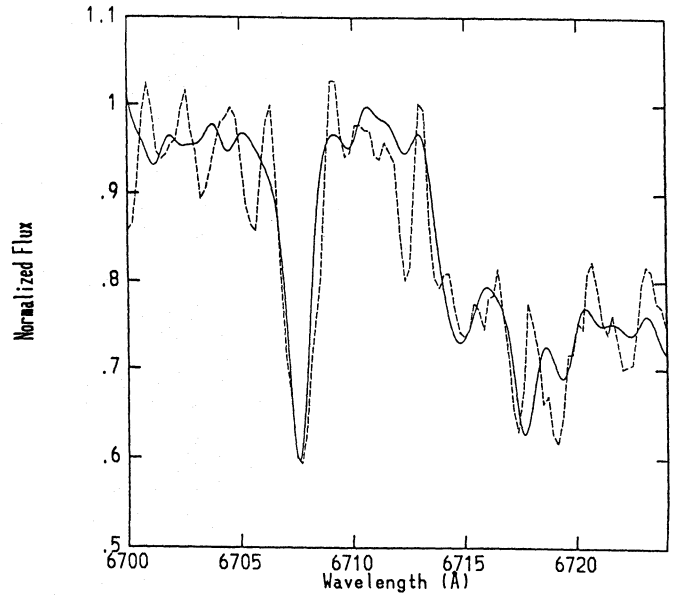


Fig. 10. LTE spectral synthesis fit to the Li I $\lambda 6708$ region of the M6 Tauri star UX Tau C. We used a model atmosphere with 3000/5.0 and $\log n(\text{Li})=1.6$

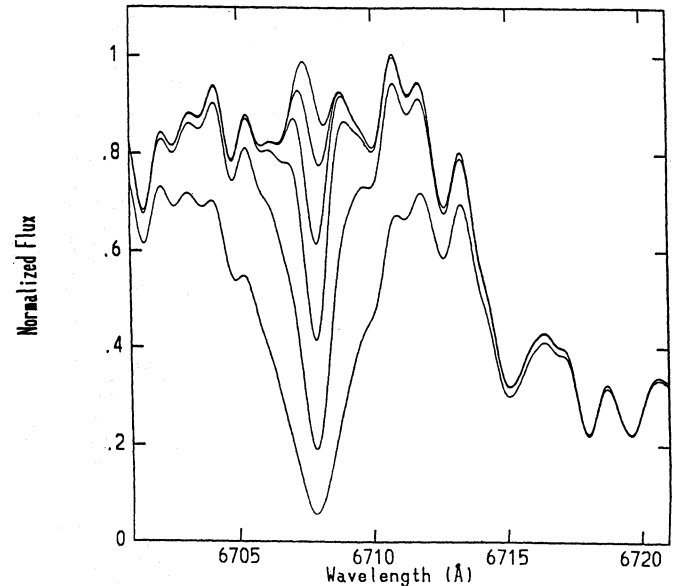


Fig. 11. Synthetic LTE Li I $\lambda 6708$ profiles for 2500/5.0 model atmosphere and $\log n(\text{Li})=3.0, 2.0, 1.0, 0.0, -1.0$ and -2.0

model atmospheres 3000/5.0, 2500/5.0, 2000/5.0 and with $v_t=2 \text{ km s}^{-1}$. First (Fig. 10), to check the reliability of the molecular data we compared with the observed spectrum of UX Tau C (Magazzù et al. 1991). We synthesized the 6700-6730 Å spectral details including the Ca I $\lambda 6718$ line + TiO γ' heads spectrum. Some modifications of the oscillator strength list was needed because the original line data gave too weak molecular absorptions in this spectral region (but we also note that part of the discrepancy could be due to inconsistencies introduced by the use of model atmospheres and spectral synthesis based on dif-

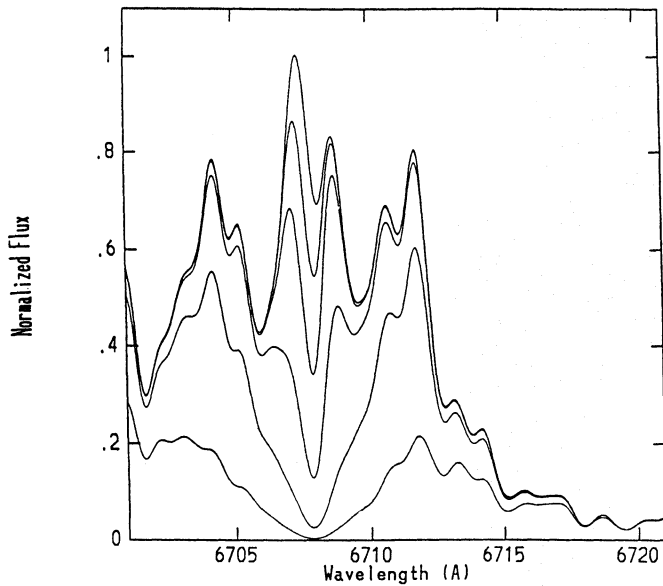


Fig. 12. Synthetic LTE Li I $\lambda 6708$ profiles for 2000/5.0 model atmosphere and $\log n(\text{Li}) = 3.0, 2.0, 1.0, 0.0, -1.0$ and -2.0

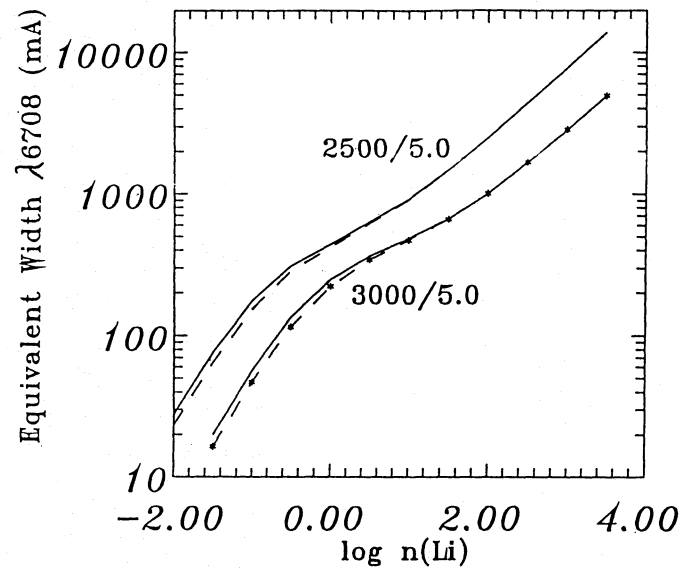


Fig. 13. LTE (solid) and NLTE (dashed) curves of growth for the Li I $\lambda 6708$ line using atmosphere models with 3000/5.0 and 2500/5.0

ferent opacities). As it can be seen in Fig. 10 the theoretical spectrum reproduces the general shape of the observational one although there are discrepancies in the position of several lines. Both, higher resolution and higher S/N observation would be desirable to improve our understanding of this spectral region.

It is clear from Fig. 11-12 that prominent Li I lines are formed. Even at $T_{\text{eff}} = 2000$ K where most of the Li in the outermost part of the atmosphere is expected to be in molecular form. Our synthetic spectra strongly suggest that Li can be observed in the spectra of the latest M-type dwarf stars. They show that the abundance of Li can be determined and that the substellar nature of brown dwarfs can in principle be established as was proposed by Rebolo et al. (1992). As a quantification of the dependence of the strength of several Li I lines on the Li abundance we show in Figs. 13-15 LTE and NLTE curves of growth for models with T_{eff} 3000 and 2500 K.

An important question (prompted by Dr. F. Allard) is the impact of the NLTE equation of state of Li on the ionization-dissociation equilibrium in the outer part of the coolest model atmospheres. Li may become an important donor of free electrons when the temperature drops below 3000 K. Indeed, for $\log N(\text{Li}) = 3.2$ the electron density in the outer part of a model atmosphere with $T_{\text{eff}} = 2500$ K and $\log g = 5.0$ is similar to the density of Li ions obtained in NLTE (see Fig. 16). The chemistry of the outer part atmosphere depends on the NLTE ionization equilibrium of elements with low ionization potential (Li, Na,...). These elements are bounded in numerous molecules making difficult the use of methods of complete linearisation. In the following, we have employed a simpler iterative algorithm already used to study the impact of NLTE on the ionization-dissociation equilibrium in the atmospheres of late-type stars (Auman & Woodrow 1975; Pavlenko 1984). In order to estimate the effect on the ionization equilibrium of Li of an increase in electron density, we

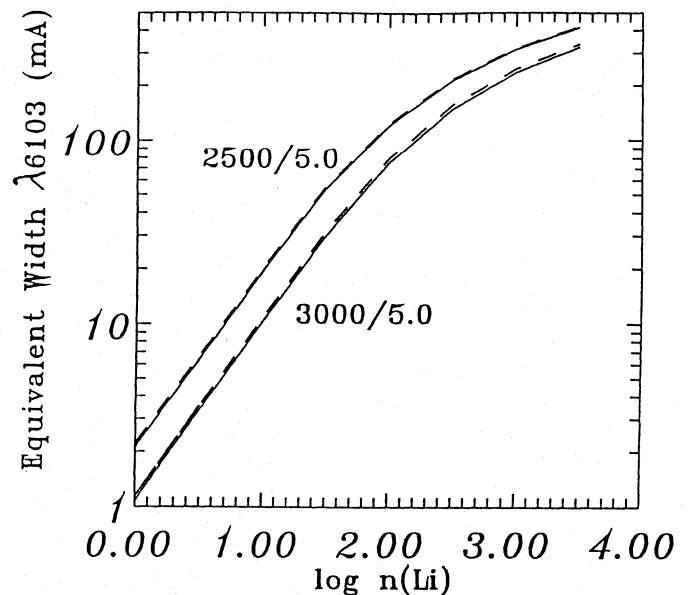


Fig. 14. LTE (solid) and NLTE (dashed) curves of growth for the Li I $\lambda 6103$ using atmosphere models with 3000/5.0 and 2500/5.0

have arbitrarily increased this density in a 2500/5.0 model atmosphere through a change of a factor 10 in the Na abundance (from $\log N(\text{Na}) = 7.32$ to 8.32). This element is not bounded with Li via direct chains of dissociation equilibrium, so the approach seems reliable. As it can be seen in Fig. 16 the increase in electronic density results in a decrease of the density of Li ions. This suggests that a self-consistent solution of the problem should not give a high contribution of Li to the electronic density. Since self-consistency would imply to solve simultaneously the NLTE ionization-dissociation equilibrium for Li and

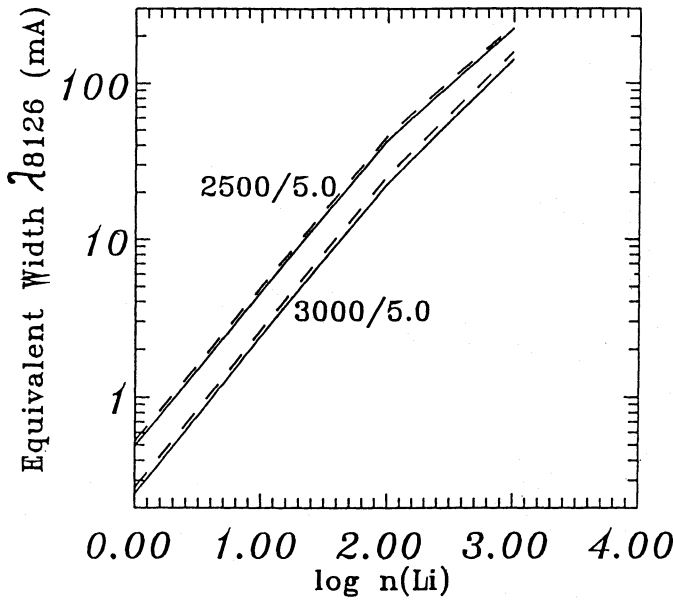


Fig. 15. LTE (solid) and NLTE (dashed) curves of growth for the Li I $\lambda 8126$ line using atmosphere models with 3000/5.0 and 2500/5.0

Na, which is beyond the frame of this paper, our NLTE results can only be considered upper limits.

4. Chromospheric-like effects on formation of Li I lines

We have done several numerical experiments aimed to test the influence of heated outermost atmospheric layers on the formation of Li I lines. The core of very strong Li I resonance lines are formed in the outer part of the atmospheres of cool dwarfs. To model the temperature structure of such atmospheric layers we used a simple procedure based on the assumption that the relation between temperature and pressure may be described by a polytropic law. Unfortunately we have no other way to model the external layers of these stars. In general, the structure of the photosphere of M-dwarfs depends mainly on convection. The convective envelope generates non-radiative energy flux which dissipates in the outer part of stellar atmospheres. Intense H_α emission has been observed in the spectra of most M-dwarfs, possibly indicating the presence of chromospheres which could heat the region where the core of the strong Li I lines are formed. Therefore, the profiles of these lines may be affected by changes in the structure of the atmospheres associated with this phenomenon.

We performed a set of computations using modified model atmospheres in which we added the chromospheric structures to the photospheres of M-dwarfs. Our modified model atmospheres consist of two different parts: One is the photosphere of the star where the continuum, weak lines and wings of strong lines are formed. We assume Kurucz or Allard models to describe the photosphere of the stars and adopt for the outermost layers a "solar-like" chromosphere. To produce this, we changed

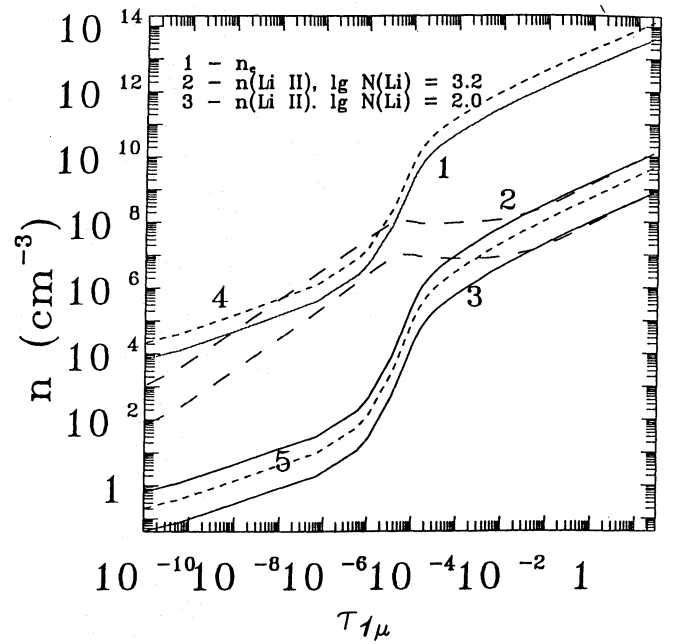


Fig. 16. Electron density (curve denoted by 1) and Li II atoms densities versus optical depth in the model atmosphere (2500/5.0/0) for $\log N(\text{Li}) = 3.2$ (curve 2) and 2.0 (curve 3). Solid lines and dashed lines show LTE and NLTE results. The curve labelled with 5 represents the LTE densities of Li II atoms computed assuming an arbitrary increase in electron density plotted as curve number 4 and obtained as explained in the text.

the structure of these outer layers modelling the increase of temperature as follows:

$$T(m) = T_{\min} + G_{\text{rad}} \times \log(m_{\min}/m) \quad (4)$$

where T and m are temperature and column mass density, $T_{\min}$ and $m_{\min}$ are the temperature and column mass densities of the "temperature minimum region", and finally G_{rad} is the gradient of temperature in the "chromosphere" of the star.

In Fig. 17 we show the temperature structure of three model atmospheres: a) is the Kurucz model 3500/4.5 without any chromosphere; b) is the previous one but modified assuming $G_{\text{rad}} = 820$, this we will termed "weak", and model c) assumes as $G_{\text{rad}} = 4000$ ("strong chromosphere"). We assume that the temperature minimum in the model atmospheres is at the depth where $\tau(1_\mu) = 10^{-4}$.

For each of the previous models, we solved the NLTE problems for a 20-levels Li I atom model and found:

a) "Weak chromosphere-like" model

The LTE and NLTE Li I $\lambda 6708$ curves of growth obtained with this model are similar to those obtained in Sect. 3.1, as it can be seen in Fig. 18. For the subordinate Li I line at $\lambda 6103$ the effect of our "weak" chromosphere is also small (see Fig. 19). We found that the NLTE equivalent widths show less sensitivity to the temperature structure than the LTE ones. In conclusion this "weak chromosphere-like" model does not produce any significant changes in both LTE and NLTE results.

b) "Strong chromosphere-like" model.

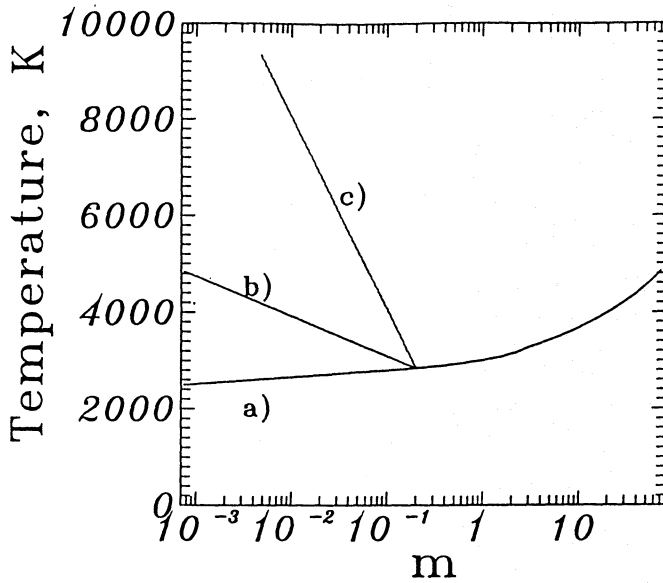


Fig. 17. Atmospheric structures (temperature vs. column mass density) of the model with 3500/4.5: *a* without chromosphere, *b* with a weak chromosphere $G_{rad}=824$, *c* with a strong chromosphere $G_{rad}=4000$. See text for details

This model produces additional continuum in the ultraviolet and the visible region which manifests in a reduction of the equivalent widths of absorption lines, this effect is similar in fact to a “veiling” of the lines. In particular, we found a dramatic change in the curves of growth computed for Li I lines both in LTE and NLTE with respect those in Sect. 3.1 (see Figs. 18 and 19). The LTE equivalent widths of the resonance Li I doublet lines decrease considerably in comparison with those obtained for the “classical” and “weak” models. The NLTE effects on the resonance Li I doublet are governed by the overionization of Li. So we have $W_{LTE} \geq W_{NLTE}$, despite W_{LTE} is decreased due to veiling produced by this “strong chromosphere-like” model. In the case of the subordinate Li I line at $\lambda 6103$ the LTE equivalent widths are decreased and NLTE effects may even produce a weak emission line.

We must note some cautions on our models and results. The models were computed under the hypothesis of hydrostatic equilibrium and the real physical conditions in M-dwarfs may be far from this assumption. For instance, stellar winds and surface inhomogeneities may play an important role. In addition, the absorption of radiation in the frequencies of bound-free lithium transitions has been computed in the LTE approach. As a result we obtain strong emission lines and some continuum emission in the UV, which could produce an excess of Li overionization. It is out of the scope of this paper to make a detailed investigation of these effects. This will be considered in a future work.

5. Conclusions

In this paper we have presented an analysis of the NLTE formation of Li I lines in the atmospheres of G-M dwarfs of solar metallicity. We solved the system of equations of statistical

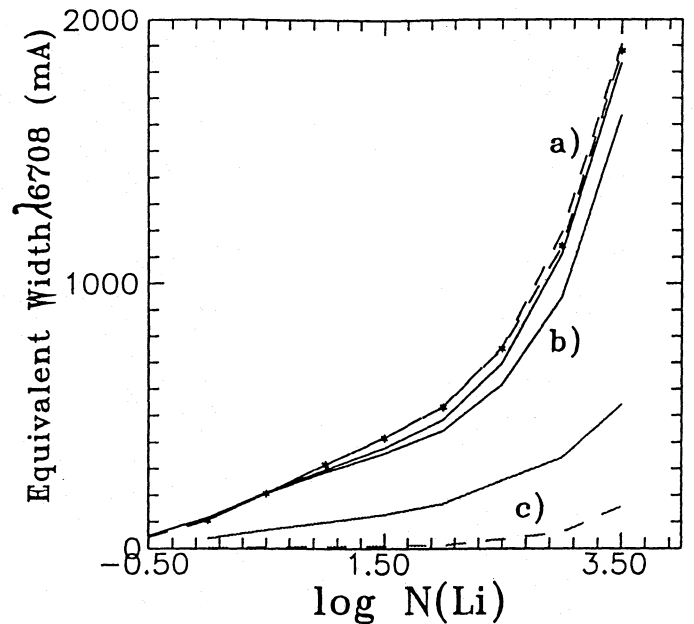


Fig. 18. LTE (solid) and NLTE (dashed) curves of growth for the Li I $\lambda 6708$ line using the models with the atmospheric structure shown in Fig. 17

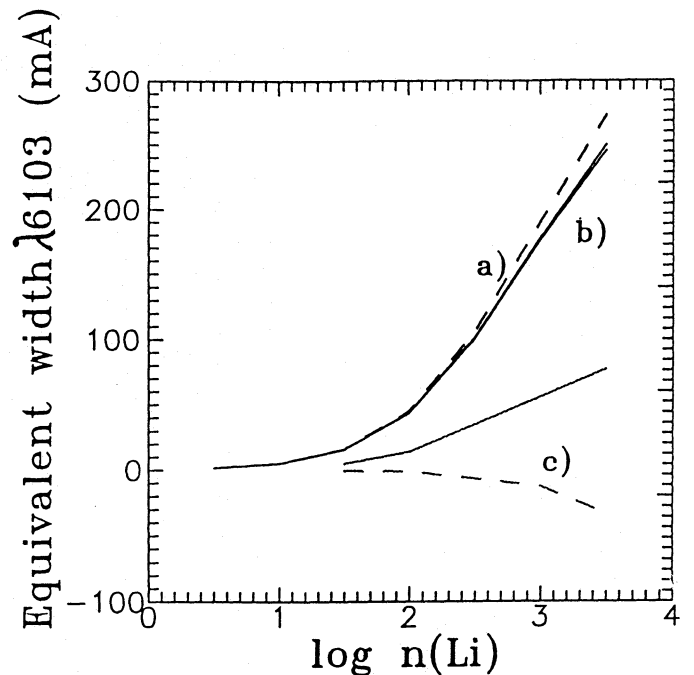


Fig. 19. LTE (solid) and NLTE (dashed) curves of growth for the Li I $\lambda 6103$ using the models with the atmospheric structure shown in Fig. 17

balance and the radiative transfer equations. Our analysis using a 20-level Li atom model showed that NLTE effects have a complicated nature. The NLTE effects are governed by the overionization of Li and by the interlocking of energy levels. As a result, the abundance corrections due to NLTE effects for a given Li I line depend on its strength and, as expected, they are different for the resonance and subordinate lines. For stars with $T_{\text{eff}} = 5500$ to 3500 K, we confirm the previous findings of Magazzù et al. (1992).

We have extended the study of the formation of Li I lines to extremely cool stellar atmospheres, including the NLTE effects and considering dissociation-ionization equilibria of Li contained species. Special attention was paid to the determination of van der Waals damping constant for the Li I lines. From the comparison of observed and synthetic spectra of cool dwarfs we found necessary to exclude damping due to molecular hydrogen from the Unsold approximation and derived an optimum correction factor of $E=2$. Our results show that prominent Li I $\lambda 6708$ lines are formed at T_{eff} in the range 3000-2000 K, even though at 2000 K most of the Li exists in molecular form in the outer atmospheric layers. This is relevant to the study of brown dwarfs. We computed the NLTE problems for Li in the atmospheres of dwarfs with $T_{\text{eff}} = 3000$ K and 2500 K, and found NLTE corrections lower than 0.1 dex.

We studied the dependence of our results on a possible “chromosphere-like” structure in the outermost layers of model atmospheres of cool dwarfs, and found that while the strength of Li I lines is not sensitive to a temperature gradient like the solar one, in the case of “strong” chromospheres, with temperature gradients several times solar, the Li I lines may be severely affected. These preliminary results stress the need for a detailed investigation of chromospheric effects on the formation of Li lines in very cool dwarfs.

Acknowledgements. We would like to thank Dr. A. Shavrina for assistance with molecular data and Dr. F. Allard for her valuable and constructive comments as referee. YaVP thanks the Instituto de Astrofísica de Canarias for hospitality during several working visits. EM acknowledges financial support from the EC Human Mobility network grant number CHRX-CT93-0329. This work was partially supported by Spanish DGICYT grant number PB92-0434-C02-01.

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