

# The formation of lithium lines in the atmospheres of super Li-rich AGB stars

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**Abstract.** The formation of lithium lines in the atmosphere of C-rich giants is discussed. LTE and NLTE approximations are used to model lithium lines in the spectra of super Li-rich AGB stars. The system of equations of the statistical balance of neutral Li in plane-parallel model atmospheres is solved for a 20-level atom model. JOLA and line-by-line models of molecular absorption are used to compute synthetic spectra as well as the opacity in the frequencies of bound-bound and bound-free transitions of the lithium lines. Curves of growth and synthetic spectra are computed in LTE and NLTE for several model atmospheres of different  $T_{\text{eff}}$  and C/O ratios for four lithium absorptions, namely: the  $\lambda 4603$ ,  $\lambda 6104$ ,  $\lambda 6708$  and  $\lambda 8126$  Å Li I lines. The sensitivity of NLTE effects on  $T_{\text{eff}}$  and the C/O ratio is discussed. We found that NLTE mainly affects the resonance line doublet ( $\lambda 6708$ ) while the impact of NLTE effects on the lithium subordinate lines, formed in the inner regions of C-rich giant atmospheres, is rather weak. Therefore the use of these lines is recommended for Li determination in AGB stars. However, in no case can we properly account for the formation of Li lines in AGB stars until sphericity, velocity stratifications, dust, chromospheres and other related phenomena, which are in fact present in AGB star atmospheres, are considered. Our results are used to derive Li abundances in three super-Li rich C-stars taking into account NLTE effects. Finally, the net Li yield from this class of stars into the interstellar medium is reconsidered.

**Key words:** stars: abundances – stars: AGB and post-AGB – stars: carbon

## 1. Introduction

The element lithium has provided many clues concerning stellar evolution and nucleosynthesis, as well as cosmology. However, its origin is still far from clear. Nowadays there is an increasing belief that this element has a multi-source nature: primordial nucleosynthesis (see the review by Wallerstein et al. 1997), galactic cosmic ray spallation in the interstellar medium and/or in the neighbourhood of supernova remnants (Meneguzzi et al. 1971; Feltzing & Gustafsson 1994), late type stars and novae

(Abia et al. 1993a; Hernanz et al. 1996), supernovae explosions (Woosley & Weaver 1995) and even spallation reactions around compact objects (Guessoum & Kazanas 1998). However, except perhaps for the Li production during the Big Bang there is no consensus about the contribution of these sources to the present cosmic abundance,  $\log \epsilon(\text{Li}) \approx 3.3$ <sup>1</sup>

The discovery of an unusually strong Li line at  $\lambda 6708$  Å by McKellar (1940) in the carbon star (C-star) WZ Cas strongly suggested that AGB stars might be an important source of Li in the galaxy. The work of McKellar was followed by similar discoveries in other AGB stars: the C-stars WX Cyg and IY Hya (Sanford 1950; Abia et al. 1991), the S-stars T Ara and T Sgr (Feast 1974; Boesgaard 1970) and the SC-stars Henize 166 and VX Aql (Catchpole & Feast 1971; Warner & Dean 1970). The same figure has also been reported in AGB stars of the Magellanic Clouds (Plez et al. 1993; Smith et al. 1995). The pioneering analysis by Cohen (1974) showed that the measured equivalent width of the  $\lambda 6708$  Å Li I line ( $W_\lambda \sim 1\text{--}10$  Å) in these stars is mainly the consequence of a strong enhancement of the lithium abundance in the atmosphere. Quantitative determinations by spectral synthesis (Denn et al. 1991; Abia et al. 1993b; Plez et al. 1993; Smith et al. 1995) have shown that the abundance of Li in these stars is 1–2 orders of magnitude higher than the present cosmic Li abundance. Therefore, these stars have been named super lithium-rich (SLiR) stars and might well constitute the main source of Li in the galaxy. The production of Li in AGB stars has received special attention in recent years (e.g. Sackmann & Boothroyd 1992). Basically, Li is produced by the reaction  ${}^3\text{He}({}^4\text{He}, \gamma){}^7\text{Be}$ , followed by  ${}^7\text{Be}(e^-, \nu){}^7\text{Li}$  in a hot convective region that brings the  ${}^7\text{Be}$  or  ${}^7\text{Li}$  to cooler regions before the  ${}^7\text{Li}$  is destroyed by  ${}^7\text{Li}(p, \alpha){}^4\text{He}$ . This is the so-called  ${}^7\text{Be}$ -transport mechanism (Cameron & Fowler 1971). Results of these theoretical studies quantitatively agree with the Li abundances derived in AGB stars of the galaxy and the Magellanic Clouds, although there are still many open questions related to the Li production in these stars. Among others we find questions about the minimum initial stellar mass which can

<sup>1</sup> The abundance of a given element X is noted as  $\log \epsilon(X) \equiv 12 + \log(N(X)/N(\text{H}))$  where  $N(X)/N(\text{H})$  is the abundance by number of the element X.

eventually become a SLiR star during the AGB phase, the duration of the SLiR phase or the actual Li yield into the interstellar medium.

Our purpose in this work is related to the reality of the Li abundances in SLiR stars and its consequences on the Li yield. At present, the uncertainty in the derivation of the Li abundances in AGB stars is not lower than 0.4–0.5 dex (see references above), mainly due to uncertainties in the stellar parameters and the fit to the observed spectra. Note, that in many situations no single set of stellar parameters is found to fit the observations. However, there are also systematic errors that are not usually taken into account that might dramatically change the Li abundance derived: uncertainties in the atmosphere models, the existence of velocity stratifications (most SLiR stars are actually variable), sphericity and NLTE effects are not currently considered as possible systematic sources of error. Of course, the consequences of each of these phenomena on Li abundance merit individual study and are beyond the scope of this work (see, however, Scholtz 1992; Jørgensen et al. 1992). Here, we will focus our attention on the effects of departures from LTE in the formation of the Li lines in C-stars.

The study of NLTE effects in the formation of lithium lines in stellar atmospheres was begun by the work of Müller et al. (1975). They performed NLTE analysis of the very weak lithium resonance line  $\lambda 6708 \text{ \AA}$  in the spectrum of the Sun. Later, Luck (1977) investigated the statistical balance of lithium in the atmospheres of G-K giants for a 4-level atom model of Li. A similar atom model was used by de la Reza & Querci (1978) and de la Reza et al. (1981). Historically, these papers considered for the first time the impact of a stellar chromosphere on the lithium lines. A new stage of research was begun with the work of Steenbock & Holweger (1984), who used the technique of complete linearization for an 8-level atom model. They studied NLTE effects in lithium lines in atmospheres of dwarfs and giants. Pavlenko (1991) considered in detail the effects of deviation from LTE in the atmosphere of red giants. Later, Magazzú et al. (1992), Martin et al. (1994) and Pavlenko (1994), continued the NLTE studies in T-Tau stars, G-K giants, subgiants and dwarfs. The main results of these studies were confirmed by the independent work of Carlsson et al. (1994), who made a similar investigation using atmosphere models with various effective temperatures, luminosities and metallicities. Finally, Houdebine & Doyle (1995), Pavlenko et al. (1995), Pavlenko & Magazzú (1996) and Martin et al. (1997) have continued the studies of different aspects of NLTE formation of lithium lines in stellar atmospheres.

As far as we know, the sole study on this subject for AGB stars is that by de la Reza & Querci (1978) who performed kinetic equilibrium calculations of neutral lithium lines in C-stars and determined the influence of the possible chromospheric radiation into the photosphere. In the present work we revise this study using up to date atomic data, collisional and radiative rates, an extended Li atom model and more reliable model atmospheres for C-stars in a wider range of effective temperatures ( $T_{\text{eff}} = 2500\text{--}3100 \text{ K}$ ) and C/O ratios (1.0–1.35) (see below). We explicitly apply our results deriving Li abundances from

synthetic spectra, both in LTE and NLTE, in three well known SLiR stars (WX Cyg, WZ Cas and IY Hya) from four accessible Li I lines: the resonance line at  $\lambda 6708 \text{ \AA}$  and the subordinate transitions at  $\lambda 4603$ ,  $\lambda 6104$  and  $\lambda 8126 \text{ \AA}$ , respectively, benefiting from high signal-to-noise ratio and high resolution spectra of these stars. The consequences on the real Li abundances in AGB stars and on their net Li yield into the interstellar medium is then reexamined.

## 2. Observations

The observations were made during 1997 and 1998 in two different observatories. We used the 4.2 m WHT at the Observatory of El Roque de los Muchachos with the Utrecht Echelle Spectrograph as the main instrument and a  $2048 \times 2048$  CCD with  $24 \mu\text{m}$  pixel size. We used the 79.0 lines/mm grating which provides less wavelength coverage, but more space between orders (20–30 arcsec). The projected size of the slit on the chip was around two pixels which gave a resolving power of 50000, the effective resolution ranging between 0.05–0.19  $\text{\AA}$  from the blue orders to the red ones. The total number of orders on the chip were 30 covering the wavelength range 0.4–1.0  $\mu\text{m}$  with some gaps between orders. WZ Cas and WX Cyg were also observed by the 2.2 m telescope at the Calar Alto Observatory. For this observational run a fibre optics cassegrain echelle spectrograph (FOCES) (Pfeiffer et al. 1998) was used. This time the chip was a  $1024 \times 1024$  Tektronik CCD with  $24 \mu\text{m}$  pixel size. The FOCES image covers the visible spectral region from 0.38 to 0.96  $\mu\text{m}$  in about 80 orders with full spectral coverage. Spectral orders are separated by 20 pixels in the blue and 10 in the red. The maximum resolving power is 40000 with a two pixel resolution element.

The reduction of the spectra was made following the standard procedures using the ECHELLE task of the IRAF software package: bias subtraction, division by flat-field images, removal of the scattered-light, extraction of the orders and wavelength calibration with Th-Ar lamps. Typically the rms in the residuals of the calibrations were better than 10 m $\text{\AA}$ . Finally, the spectra were divided by the spectrum of a hot rapidly rotating star to remove telluric absorptions, although they are only important in the  $\lambda 8126 \text{ \AA}$  range. The signal-to-noise ratio of the spectra vary along the wavelength, from  $S/N \sim 20$  in the bluest orders to  $S/N \sim 700$  around  $\lambda 8000 \text{ \AA}$ . Since our stars are relatively bright objects ( $V \sim 7\text{--}11$ ), this strong variation in the S/N ratio achieved is mainly due to the very low emissivity of the stars below  $\lambda \sim 4500 \text{ \AA}$ . This is particularly evident in IY Hya, which is an extremely red object. For this reason, its spectrum in the  $\lambda 4603 \text{ \AA}$  range is of too low quality ( $S/N \sim 30$ ) and has not been considered.

## 3. The abundance analysis

### 3.1. Atomic and molecular line lists

The line list described in Lèbre et al. (1999) completed with  $C_2$  lines has been used for the analysis of the  $\lambda 6708 \text{ \AA}$  region. Lines from the  $^{12}C_2$ ,  $^{12}C^{13}C$  and  $^{13}C_2$  Swan system (Kurucz

CD ROM no 23) were considered and from the Phillips red system were predicted as in de Laverny & Gustafsson (1998). The line lists for the  $\lambda 4603$ ,  $\lambda 6104$  and  $\lambda 8126$  Å spectral domains were built in a similar way for the C<sub>2</sub> and CN molecules, and atomic line data were found in VALD (Piskunov et al. 1995). The broadening by radiation and van der Waals damping were calculated as in de Laverny & Gustafsson (1998). Line data were adjusted as described in Lèbre et al. (1999) by comparison with the solar spectrum using the Holweger & Müller (1974) model atmosphere for the Sun with element abundances from Anders & Grevesse (1989). A good fit to the solar spectrum was obtained in the  $\lambda 6708$  and  $\lambda 8126$  Å spectral domains in  $\sim 50$  Å around the corresponding Li line. The fit, however, was not as good in the other two spectral ranges. Indeed, in the  $\lambda 4603$  and  $\lambda 6104$  Å regions there are a number of unidentified features in the solar spectrum with a modest absorption ( $\sim 5$ – $25$  mÅ). Most of these features could be atomic in nature because no such intense molecular absorptions are expected in the Sun in these spectral ranges. However, we did not find any atomic lines in the data base of VALD or of Kurucz (1998) at the wavelengths of the missing features. Nevertheless, we were able to obtain a good fit to the solar spectrum in at least  $10$  Å around the  $\lambda 4603$  Å and  $\lambda 6104$  Å Li I features. Thus, we do not believe this problem will introduce an additional source of error into the abundance of Li derived from these two spectral domains.

### 3.2. Atmospheric parameters

Stellar parameters for the stars studied were taken from the literature when available. For WX Cyg the effective temperature derived by Ohnaka & Tsuji (1996) from the infrared flux method (IRFM) was adopted. For WZ Cas, effective temperature derived from the IRFM and angular radii measurements (Dyck et al. 1996) agree quite well ( $\pm 30$  K). However, the value derived from these two methods (3150 K) contrasts with that derived from infrared photometry ( $\sim 2800$  K; see Noguchi et al. 1981; Frogel & Hyland 1972). We adopted here the value obtained by Dyck et al. (1996). For IY Hya there is no estimate of its effective temperature nor its photometry is available in the literature. We estimated the effective temperature by comparing its spectrum with the temperature sequence spectral atlas for C-stars created by Barnbaum et al. (1996). From that comparison we believe that IY Hya is a cool N-star and consequently, we adopted the lower effective temperature in our grid of atmosphere models i.e.:  $T_{\text{eff}} = 2500$  K. The uncertainty in  $T_{\text{eff}}$  is, however, no less than  $\pm 200$  K; it might well be larger for IY Hya. Note also that these stars are variable and we suspect  $T_{\text{eff}}$  variations as large as  $\sim 300$  K during their cycle (see Richichi et al. 1995). The consideration of an unique effective temperature for these stars is therefore a strong assumption.

A solar metallicity ( $[\text{Fe}/\text{H}]=0.0$ ) was considered for the three stars. Most galactic C-stars are of Population I with near solar metallicity although typically they show strong enhancements of heavy elements (Zr, Ba, La etc...)(Utsumi 1985; Dominy 1985). We checked that there is no intense heavy element line close enough to the four Li absorptions in our line

**Table 1.** Log of the observations and stellar parameters

Star	Spec. type	Var. type	$T_{\text{eff}}$	C/N/O	$^{12}\text{C}/^{13}\text{C}$
WX Cyg	C8,2eJ	M	2990	8.93/7.99/8.92	4.8
WZ Cas <sup>a</sup>	C9,2J	SRa	3140	8.932/7.99/8.92	5.0
IY Hya	N	?	2500	8.93/7.99/8.92	26

<sup>a</sup> WZ Cas has also been classified as a SC-type star.

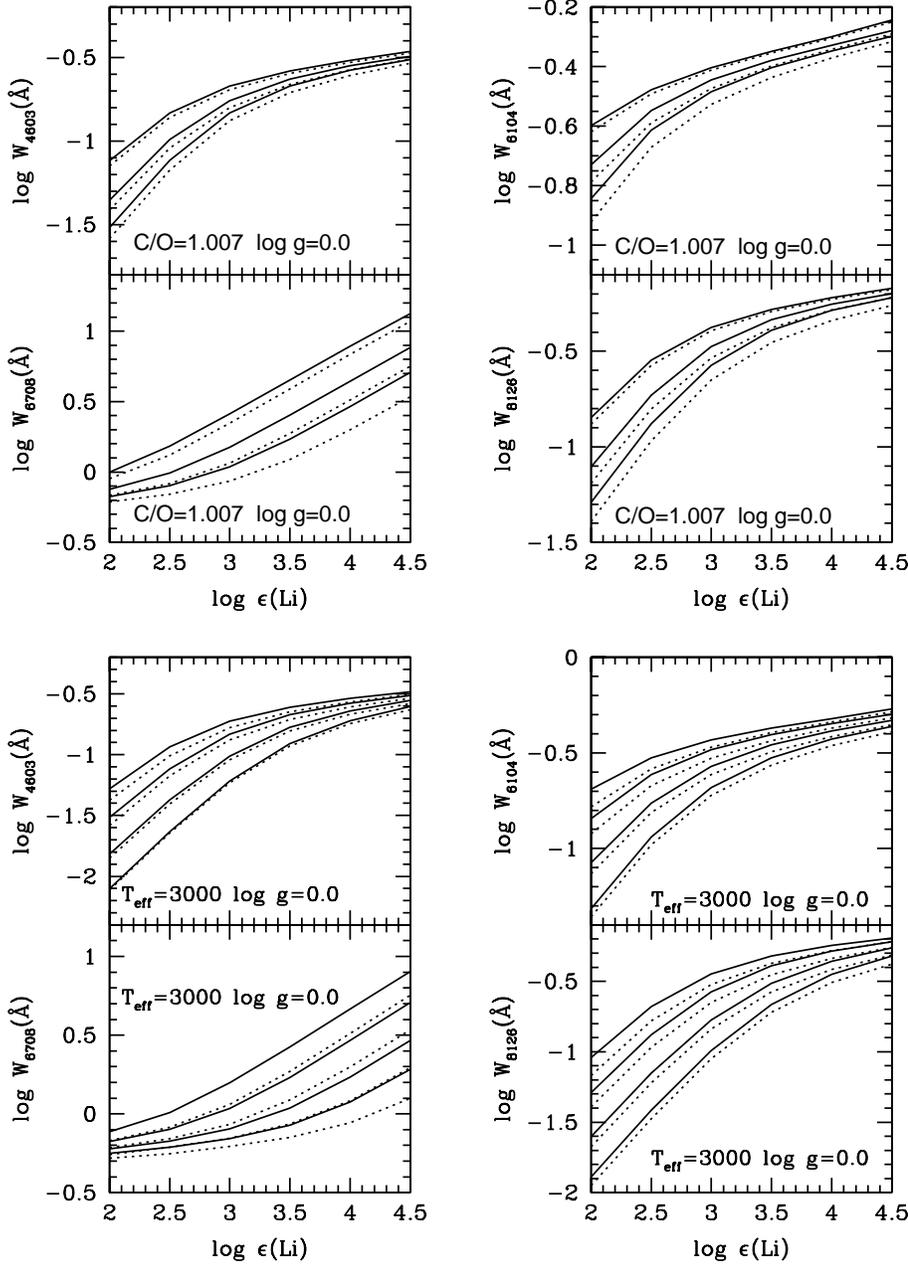
lists that may affect the Li abundance derivation. A study of the heavy element enhancements in the SLiR stars and other normal C-stars will be presented in a separate work.

A gravity of  $\log g = 0.0$  and a microturbulence parameter of  $\xi = 2.5 \text{ km s}^{-1}$  were adopted. These are typical values for C-stars (see Lambert et al. 1986). Concerning gravity, note that studies by Pavlenko (1990) and Magazzú et al. (1992) on O-rich dwarfs, subgiants and giant stars showed no important sensitivity in the ratio of LTE/NLTE Li abundances caused by changes in the gravity of  $\Delta \log g = \pm 1$ , especially in the case of strong lines. Thus, uncertainties in gravity should play a minor role in the formation of the lithium lines in C-rich atmospheres. Radiative damping (which does not depend on  $\log g$ ) plays the main role in the formation of the wings of the saturated lithium lines. More serious seem to be the consequences of changes in the temperature structure of the atmosphere with decreasing gravity due to the increase in the effectiveness of sphericity effects. However, analysis of these effects lies beyond the scope of this paper.

Finally, a model atmosphere was interpolated in  $T_{\text{eff}}$  and the C/O ratio for each star from an unpublished grid of models for C-stars (Eriksson et al., private communication). These models are constructed under the basic hypotheses of hydrostatic equilibrium and plane-parallel approximation. The models include more complete opacity data of HCN and C<sub>2</sub>H<sub>2</sub> (in addition to diatomic molecules) with the sampling treated by an opacity distribution function (see Eriksson et al. 1984, for details). The final C/O ratio of the model atmosphere used in the spectral synthesis was obtained by an iterative procedure comparing synthetic and observed spectra until a good fit was obtained. Li lines were not included in this procedure. However, the same C/O ratio was not found to give the best fit in the four spectral domains for a given star, although differences in the C/O ratio never exceeded a few hundredths. For instance, in the  $\lambda 4603$  and  $\lambda 6104$  Å regions we systematically derived a lower C/O ratio by  $\sim 0.03$  hundredths. Table 1 shows the log of the observations and the final stellar parameters used in the analysis. The quoted CNO abundances are the mean values of those obtained from the best fit for each spectral domain (N abundance plays a minor role).

### 3.3. LTE abundances

Lithium abundances were derived by synthetic spectra calculated with a modified version of the code written at the Uppsala Astronomical Observatory. The theoretical spectra were convolved with the corresponding FWHM to match the instrumental profile in the four spectral domains following the pro-



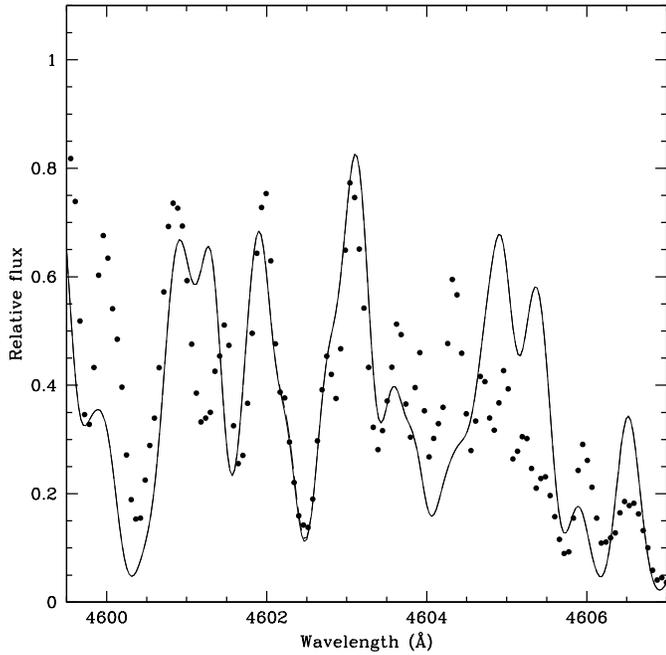
**Fig. 1.** Theoretical LTE (solid) and NLTE (dotted) curves of growth for the four Li I absorptions for different  $T_{\text{eff}}$ . The pairs of curves (solid-dotted) from top to bottom in each plot are for  $T_{\text{eff}} = 2500, 2800$  and  $3000$  K, respectively.

**Fig. 2.** Theoretical LTE (solid) and NLTE (dotted) curves of growth for the four Li I absorptions for different C/O ratios. The pairs of curves (solid-dotted) from top to bottom in each plot are for C/O = 1.007, 1.02, 1.1 and 1.35, respectively.

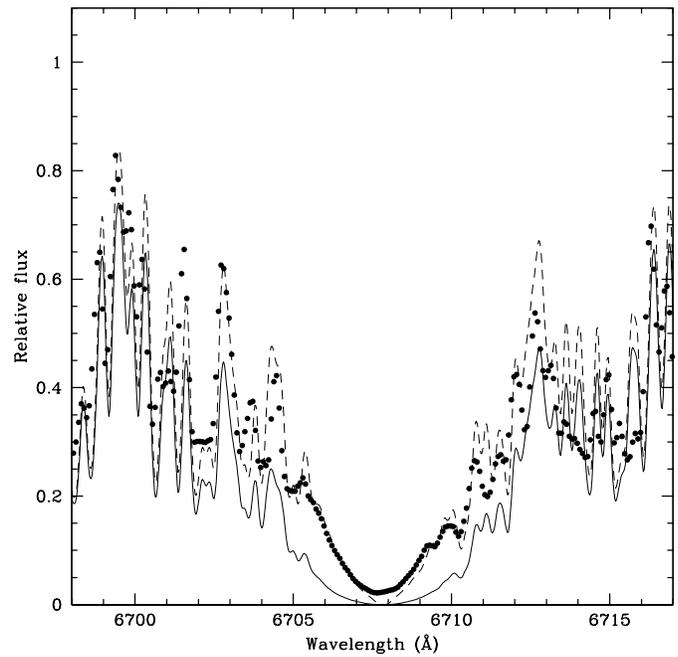
cedure used in Abia et al. (1993b). The carbon isotopic ratios ( $^{12}\text{C}/^{13}\text{C}$ ) derived in Abia & Isern (1997) from spectral synthesis to the  $^{12}\text{CN}$  and  $^{13}\text{CN}$  lines in the  $\lambda 7990\text{--}8030$  Å spectral region were adopted (see also Abia & Isern (1996) and de Laverny & Gustafsson (1998), for details on the analysis and the choice of the CN parameters, respectively). Table 1 shows the carbon isotopic ratio adopted in the stars. They are in fair agreement with those derived by Ohnaka & Tsuji (1996) and Lambert et al. (1986) in WX Cyg and WZ Cas. The total error due to stellar atmosphere parameter uncertainties, continuum placement and the fit itself amount to  $\pm 0.4\text{--}0.5$  dex for Li (LTE) abundances and  $\pm 6\text{--}13$  for the  $^{12}\text{C}/^{13}\text{C}$  ratio (see references above).

Figs. 1 and 2 (solid lines) show the behaviour with  $T_{\text{eff}}$  and the C/O ratio of curves of growth calculated in LTE for the four

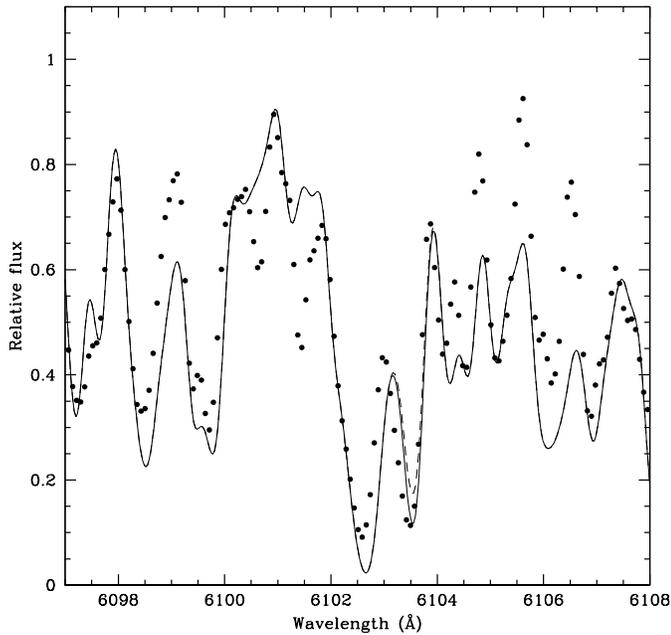
Li absorptions. As can be clearly seen, subordinate lines are saturated for high Li abundances ( $\log \epsilon(\text{Li}) > 3$ ). For the resonance line, however, the Li absorption increases more steeply with increasing Li abundance. For very high Li abundances ( $\log \epsilon(\text{Li}) > 4$ ), the subordinate lines are not very sensitive to the effective temperature, the C/O ratio or gravity (as mentioned before). This is a consequence of their saturated behaviour. The opposite occurs with the resonance line. This might lead us to consider the resonance line the better tool for abundance determinations in C-stars. However, the resonance line forms in the outermost layers (see below) where the atmosphere structure is quite uncertain in C-stars and the microturbulence may even become supersonic. We will also see that NLTE effects are much larger for this transition.



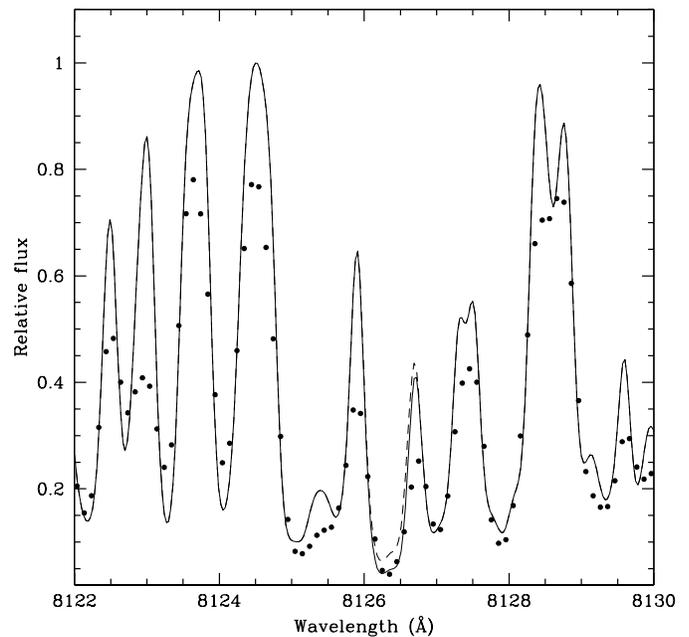
**Fig. 3.** Synthetic spectral fit to the  $\lambda 4603 \text{ \AA}$  spectral domain in WZ Cas for  $\log \epsilon(\text{Li})=3.0$ . Note the strong discrepancy between observed (dots) and synthetic spectra in LTE (solid) and NLTE (dashed) (LTE and NLTE fits to the Li line almost coincide). Most of this discrepancy is probably due to an incorrect continuous opacity in this spectral range. The Li abundances derived from this line were not considered.



**Fig. 5.** As Fig. 4 in the  $\lambda 6708 \text{ \AA}$  spectral domain of WZ Cas for  $\log \epsilon(\text{Li})=5.0$



**Fig. 4.** Synthetic spectral fit to the  $\lambda 6104 \text{ \AA}$  spectral domain of WZ Cas for  $\log \epsilon(\text{Li})=3.0$  LTE (solid line), NLTE (dashed line), observed spectrum (dots).



**Fig. 6.** As Fig. 4 in the  $\lambda 8126 \text{ \AA}$  spectral domain of WZ Cas for  $\log \epsilon(\text{Li})=4.5$

Figs. 3 to 6 show synthetic fits in LTE to the different spectral domains in WZ Cas. Synthetic spectra agree quite well with the observations for the  $\lambda 6708$  and  $\lambda 8126 \text{ \AA}$  regions but this is not

the case for the  $\lambda 4603$  and  $\lambda 6104 \text{ \AA}$  ones. Some of the discrepancy is certainly due to the missing features in our line lists as mentioned in 3.1. Moreover, in the  $\lambda 4603$  and  $\lambda 6104 \text{ \AA}$  regions

we obtain systematically larger residual fluxes than observed. This, by the way, means that the Li abundances derived from the  $\lambda 4603$  and  $\lambda 6104$  Å Li lines are systematically lower (see Table 3) than those derived from the red Li lines. The same figure was found by de la Reza & da Silva (1995) studying the formation of Li lines in K-giant stars. The reason for this is unknown. Bad  $gf$ -values for  $C_2$  lines, which are numerous in these bluest spectral regions, might partially explain this problem. Note that in these two spectral domains most of the  $C_2$  lines were taken from the data compilation by Kurucz, which is probably not very accurate. Note also that we were not able to check their  $gf$  values with the solar spectrum as mentioned above. The discrepancy between theoretical and observed fluxes is particularly evident in the  $\lambda 4603$  Å region. We confirmed that most of the strong absorptions in this spectral range are due to atomic lines while molecular lines contribute most to the background absorption. However, no reasonable reduction of the metallic abundances in the star can solve this discrepancy. Therefore, we are led to believe that an incorrect figure for continuous opacity might be the main cause of this.

The problem of the missing opacity in the blue has been widely discussed in the literature. Recently there have been some new results in this sense. Yakovina & Pavlenko (1998) showed that to fit the head of the strong NH band  $A^3\Pi - X^3\Sigma^-$  at  $\lambda 336$  nm in the spectrum of the Sun, one should increase the continuum absorption coefficient in the region by a factor  $\kappa_\nu \sim 1.7-1.9$ . Recently, Bell & Balachandran (1998) increased  $\kappa_\nu \sim 1.6$  to fit Be II lines at  $\lambda 313.0$  nm in the solar spectrum. We tried to artificially simulate this missing opacity by increasing the  $H^-$  opacity by a free factor (namely, increasing the electronic pressure by a factor  $\sim 3$ ). Indeed, in this case theoretical residual fluxes are lower (except for the very strong (saturated) lines) and the agreement between observed and theoretical spectra improve. We preferred, nevertheless, to be coherent in our analysis in the four spectral domains and did not artificially change our set of conventional opacity sources. Thus, we used the same model atmosphere for all the spectral ranges and decided, for that reason, not to consider Li abundances derived from the  $\lambda 4603$  Å range. We will have to wait for the next generation of atmosphere models for C-stars to study this problem better (Plez et al. 1999). Note that in principle sphericity effects should be more pronounced in the blue part of the spectrum because here the sensitivity to the temperature structure is higher even for strong spectroscopic features formed in the outer atmosphere.

On the other hand, this discrepancy may be caused (at least partially) by the impact of dust opacity on the star's spectrum. Indeed, the formation of dust in the atmosphere of AGB stars and their envelopes has been known for a long time (see references in Wallerstein & Knapp 1998). Dust particles can contribute to total opacity via scattering processes, i.e. with cross-sections  $\sim 1/\lambda^n$ . In that case the contribution of the dust opacity would increase to the blue. Li-rich K-giants also show a red excess, probably caused by a dusty envelope (although of a different nature; de la Reza & da Silva 1995). One may propose other explanations to explain this effect. For instance, the procedure

**Table 2.** Data for JOLA opacities used in this work

Molecule	System	$gf$	$\lambda_1$ (nm)	$\lambda_2$ (nm)	System names
CaO	$C^1\Sigma-X^1\Sigma$	0.080	730.0	923.0	
CS	$A^1\Pi-X^1\Sigma^+$	0.011	240.0	330.0	
$C_2$	$e^3\Pi_g-a^3\Pi_u$	0.007	237.0	328.5	Fox-Herzberg
$C_2$	$A^1\Pi_u-X^1\Sigma_g^+$	0.011	672.0	1549.0	Phillips
$C_2$	$b^3\Sigma_g^- - a^3\Pi_u$	0.002	1100.0	2700.0	Ballik-Ramsay
$C_2$	$d^3\Pi_g-a^3\Pi_u$	0.033	340.0	785.0	Swan
CO	$B^1\Sigma^+-A^1\Pi$	0.021	412.0	662.0	Ångström
CO	$C^1\Sigma^+-A^1\Pi$	0.022	368.0	571.0	Herzberg
CO	$A^1\Pi-X^1\Sigma^+$	0.12	114.0	280.0	
SO	$A^3\Pi-X^3\Sigma^-$	0.21	246.0	380.0	
SiO	$E^1\Sigma^+-X^1\Sigma^+$	0.330	171.5	200.0	
SiO	$A^1\Pi-X^1\Sigma^+$	0.16	207.0	330.0	
NO	$C^2\Pi_r-X^2\Pi_r$	0.0150	207.0	275.0	$\delta$
NO	$B^2\Pi_r-X^2\Pi_r$	0.0035	200.0	380.0	
NO	$A^2\Sigma^+-X^2\Pi_r$	0.0020	195.0	340.0	$\gamma$
MgO	$B^1\Sigma^+-X^1\Sigma^+$	0.048	454.0	544.0	
CN	$A^2\Pi-X^2\Sigma^+$	0.0011	400.0	5630.0	Red
CN	$B^2\Sigma^+-X^2\Sigma^+$	0.036	240.0	600.0	Blue
AlO	$C^2\Pi_r-X^2\Sigma^+$	0.040	200.0	400.0	
AlO	$B^2\Sigma^+-X^2\Sigma^+$	0.039	404.0	580.0	

$\lambda_1$  and  $\lambda_2$  are the limits for the molecular band opacity computations. Frank-Condon factors are from Kuz'menko et al. (1984) and  $gf$  values from Kuzmetzova et al. (1980).

used to place the continuum level in the observed spectrum still seems very subjective. To provide more balanced conclusions regarding this problem we suggest that a more detailed study of these regions should be carried out in several SLiR stars.

### 3.4. NLTE procedure

To carry out the NLTE analysis for a 20-level Li atom model, we followed the procedure described in Pavlenko (1994) and Pavlenko & Magazzú (1996). A few specific items were taken into account here:

- ionization-dissociation equilibria were computed for the carbon-rich case, i.e. considering C-contained molecules formation: CO, CH, CN,  $C_2$ , CS, HCN,  $H_2C$ ,  $H_3C$ ,  $H_4C$ ,  $HC_2$ ,  $H_2C_2$  and  $HC_3$ .
- in the frequencies of bound-free transitions of Li I the opacity of diatomic molecules was computed in the framework of just-overlapping-line approximation (JOLA, see Table 2).
- in the frequencies of bound-bound linearized transitions of Li I the atomic absorption was included. Furthermore, in the frequencies of the four Li lines we considered the absorption of CN and  $C_2$  for a given  $^{12}C/^{13}C$  ratio (see Table 1).

The most relevant work to the present study was done by de la Reza & Querci (1978; thereafter RQ). Using a divergence flux method these authors carried out an extensive modelling of NLTE effects of lithium lines in C-stars. They used a 4 level lithium atom model, atmosphere models by Querci et al. (1974) and Johnson (1974) with effective temperatures of 3800, 3600 and 3500 K (warmer than the  $T_{\text{eff}}$  values usually derived in C-N stars), gravity  $\log g = 1.0$ , C/O = 1.3 and modelled three Li I lines, namely the  $\lambda 6104$ ,  $\lambda 6708$  and  $\lambda 8126$  Å lines. They also

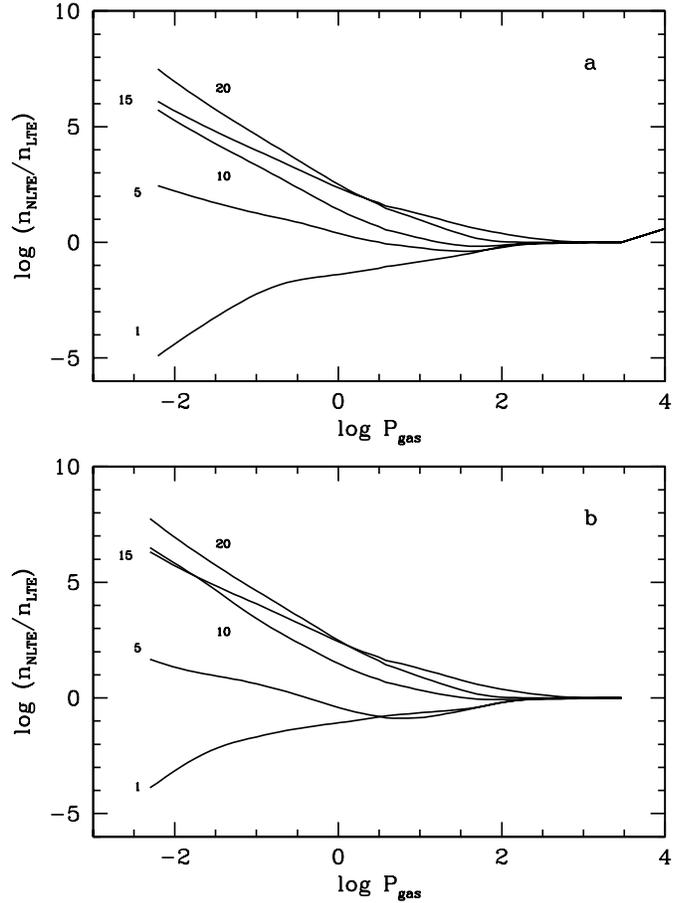
tried to model the impact of a chromosphere on the formation of lithium lines using the approach of *radiative temperature* ( $T_{\text{rad}}$ ) on the bound-free transitions of lithium. Several aspects in their NLTE calculation differ from the present study:

1. *The atom model.* We used a 20-level atom model, which allowed us to consider the interlocking of lithium lines (transitions) more appropriately. The ionization equilibrium of lithium is formed by the whole system of the bound-free transitions. However, as noted by RQ (see also Pavlenko 1991), transitions from/on the second level play the main role.
2. *Bound-free transitions.* The radiation field in bound-free transition computations is very important in the modelling of lithium lines without LTE. Indeed, the effectiveness of the overionization of lithium depends directly on the mean intensities of the radiation field in the blue part of the spectrum (Pavlenko 1991). The approximation  $T_{\text{rad}} = T_e$  (*electronic temperature*) used by RQ does not produce any overionization of lithium. Only in the case of  $T_{\text{rad}} > T_e$  does the ionization of lithium increase with respect to the LTE case. Note that  $T_{\text{rad}} > T_e$  was considered by RQ only when a chromospheric radiation field was included. As noted by these authors, this approximation seems to be rather crude for the radiation field.
3. *bound-bound transitions.* Lithium lines were treated by RQ as singlets. Basically, radiation transfer in the frequencies of several multiplet lines should differ from the case one single (strongest) line. Moreover, we include molecular line absorption in the continuous (background) opacity. In principle, this should reduce the probability of photon losses from the atmosphere, i.e. it directly affects the processes of radiative transfer. On the other hand, the radiative transfer in the continuum differs substantially from the case of continuum+lines in an atmosphere with chromosphere, as here the impact of the hot chromospheric layers on the photosphere might be weaker.

### 3.5. NLTE curves of growth, synthetic spectra and abundances

Computations of LTE and NLTE curves of growth and synthetic spectra were performed by using a modified version (see Pavlenko 1999) of the code WITA2 (Pavlenko & Magazzú 1996)<sup>2</sup>. The dependence of the departure coefficients  $b_i = N_{\text{NLTE}}^i / N_{\text{LTE}}^i$ , where  $N_{\text{NLTE}}^i$  and  $N_{\text{LTE}}^i$  are the NLTE and LTE populations of the  $i$  level, upon the depth in a typical C-star atmosphere is shown in Fig. 7. The behaviour of the departure coefficients of lower and upper lithium levels differ substantially. The populations of the lower levels are reduced by the overionization processes. On the contrary, upper levels are overpopulated relative to the LTE case because they are more closely linked with the continuum (see also Pavlenko 1994, Carlsson et al. 1994, Pavlenko & Magazzú 1996). Indeed, for  $\log \epsilon(\text{Li}) >$

<sup>2</sup> Comparison between LTE abundances derived with this code and those obtained with the Uppsala's code showed an excellent agreement ( $\sim \pm 0.01$  dex).



**Fig. 7.** **a** Departure coefficients of five Li levels in the atmosphere of a  $T_{\text{eff}}/\log g/(C/O) = 3000/0.0/1.007$  C-star computed with a lithium abundance of  $\log \epsilon(\text{Li}) = 3.0$ . **b** The same for  $\log \epsilon(\text{Li}) = 4.5$ .

4.0 the departure coefficients of the first level become very low in the outermost layers ( $b_1 < 10^{-4}$  at  $P_g < 0.01$ ), where the NLTE core of the Li resonance line forms.

On the other hand, the depth of formation of lithium resonance and subordinate lines is quite different. For large lithium abundances ( $\log \epsilon(\text{Li}) > 4.0$ ) the formation region for the resonance line shifts toward the outermost layers, where the temperature drops below 1000 K. In fact, we have to extrapolate the model atmosphere structure to  $\log P_{\text{gas}} \approx -5$  to take the line formation consistently into account. This produces additional problems in the computation of collisional and radiative rates. Here we are approaching the interstellar medium regime, where our approximations for collisional and radiative rates may not be valid. Moreover, in this regime the splitting of Li terms into sublevels may also become important although, since we are dealing with saturated lines, we believe that this effect is not critical. Lithium subordinate lines are formed in deeper layers. For instance, even for  $\log \epsilon(\text{Li}) > 4.5$  the core of the  $\lambda 6104 \text{ \AA}$  doublet forms in a region with temperature  $\sim 2000 \text{ K}$ . As a consequence, the NLTE formation regime of this Li line changes dramatically: the interlocking processes of radiative transitions (see Magazzú et al. 1992; Carlsson et al. 1994) become more

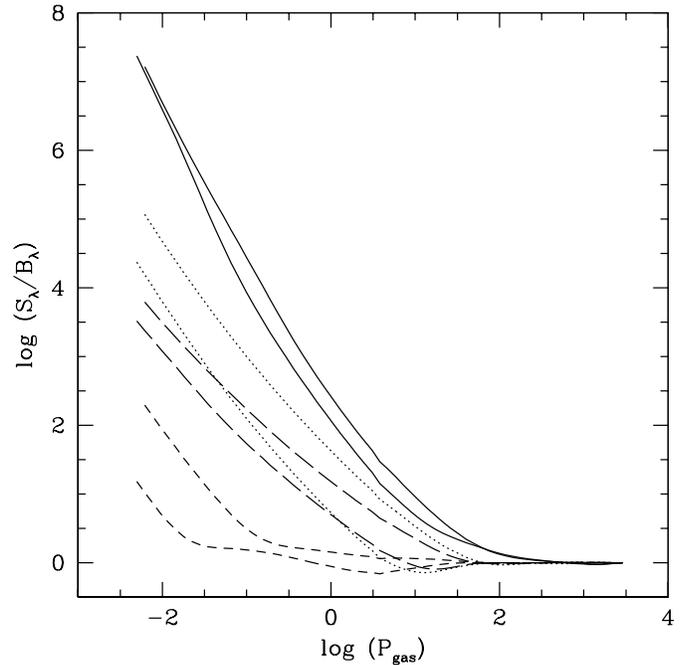
**Table 3.** LTE/NLTE lithium abundances in the stars studied

Star	$\lambda 6104 \text{ \AA}$		$\lambda 6708 \text{ \AA}$		$\lambda 8126 \text{ \AA}$	
	LTE	NLTE	LTE	NLTE	LTE	NLTE
WX Cyg	3.2	3.5	3.7	4.0	4.2	4.4
WZ Cas	3.1	3.3	4.5	5.0	4.6	4.8
IY Hya	2.6	2.7	2.5	2.7	3.2	3.3

important than overionization. In this situation, line profiles depend on the behaviour of the source function which is affected by the whole set of radiative transitions. In brief, considering the formation of lines in the outermost layers we note: i) the opacity here drops sharply due to the low molecular and  $H^-$  density, ii) the electron density is low and its effect on collision rates is small and iii) the electron temperature is also low, so that the effectiveness of the overionization  $\propto e^{-(T_e - T_{\text{rad}})/kT}$  would be high.

Figs. 1 and 2 (dashed lines) also show theoretical NLTE curves of growth for the four Li lines. Departures from LTE are very important for the resonance  $\lambda 6708 \text{ \AA}$  line. NLTE corrections for this line can amount to 0.6 dex! However, NLTE effects for the subordinate lines are weak ( $\leq 0.2$  dex) and even decrease for strong Li absorptions (high Li abundances,  $\log \epsilon(\text{Li}) \geq 4$ ). We also see from these figures that NLTE effects decrease for decreasing  $T_{\text{eff}}$  and increasing C/O ratio in the model atmosphere. When  $T_{\text{eff}}$  drops the opacity of the carbon-contained molecules increases so that the difference between  $T_{\text{rad}}$  (of the radiation field in the bound-free frequencies of Li) and  $T_e$  decreases. The same holds when the C/O ratio increases in the atmosphere. It is interesting to note that LTE/NLTE abundances converge for high Li abundances for the subordinate lines whatever the  $T_{\text{eff}}$  and/or the C/O ratio in the atmosphere. This gives us a chance to use subordinate lines as a tool for deriving Li abundances in Li-rich AGB stars even in the LTE approach, despite their saturated nature. Figs. 3 to 6 show synthetic fits in NLTE (only for Li lines; i.e. dashed lines) in our stars. The difference between the LTE/NLTE fits to the resonance line is remarkable. For the subordinate lines, LTE and NLTE fits differ only slightly.

Table 3 shows the final NLTE Li abundances derived in our stars. NLTE corrections are always positive, ranging from 0.1 to 0.5 dex. As was shown by Magazzú et al. (1992) for the case of G-M stars with solar abundances, the significance of NLTE effects depends upon the line strength. Li lines of moderate intensity ( $W_\lambda > 0.2 \text{ \AA}$ ) form in a region where  $S_\nu(\tau_{\text{NLTE}} \approx 1) < B_\nu(\tau_{\text{LTE}} \approx 1)$ . The NLTE cores of the resonance doublet become stronger than the LTE ones and, as a result, NLTE abundance corrections  $\Delta \log \epsilon(\text{Li}) = \log \epsilon(\text{Li})_{\text{NLTE}} - \log \epsilon(\text{Li})_{\text{LTE}}$  are negative. However, in the case of the strongest (saturated) Li resonance doublets the difference between LTE and NLTE cores cannot be large (because both approach to zero) then, NLTE corrections again become positive as in the case of weak lines. Note that there is a region in the atmosphere where  $S_\nu < B_\nu$  holds for all except the  $\lambda 4603 \text{ \AA}$  line (Fig. 8) in the case of intermediate strong lines ( $\log \epsilon(\text{Li}) \sim 3$ ). In these regions the interlocking processes of Li radiative transitions play the main role.



**Fig. 8.**  $S_\nu/B_\nu$  ratio for the four Li lines in the atmosphere 3000/0.0/1.007 of a C-star for different lithium abundances. Curves correspond to the  $\lambda 4603$  (solid),  $\lambda 6104$  (dotted),  $\lambda 6708$  (long dashed) and  $\lambda 8126 \text{ \AA}$  (short dashed) Li lines, respectively. For each pair of curves the upper line is computed with  $\log \epsilon(\text{Li})=3.0$  and the lower one with  $\log \epsilon(\text{Li})=4.5$ .

#### 4. Discussion and conclusions

We now compare our LTE/NLTE results with the literature. Abia et al. (1991) derived Li abundances in the same stars using the  $\lambda 6708 \text{ \AA}$  Li line. The abundances obtained here are considerably lower. In WZ Cas and WX Cyg the differences can be ascribed to the different choice of  $T_{\text{eff}}$  and the C/O ratio in the model atmosphere but also to the more complete molecular line list used in this work, which makes the background absorption more intense in the  $\lambda 6708 \text{ \AA}$  region. Note that Abia et al. (1991) did not include the  $C_2$  molecule (in any isotopic form) or the  $^{13}\text{CN}$  molecule in their line list. In IY Hya, moreover, the spectrum now analyzed in the  $\lambda 6708 \text{ \AA}$  range shows a much less intense Li line than that from which the Li abundance was derived by these authors:  $W_{6708} \sim 2.5 \text{ \AA}$  here against  $7.5 \text{ \AA}$  in Abia et al. (1991). A similar variation in time might be present in the spectrum of WX Cyg analyzed here ( $4.5$  vs.  $6.5 \text{ \AA}$ ). Whether this variation is an effect of a varying  $T_{\text{eff}}$  along the pulsational phase or just evidence of the time scale for Li formation/depletion in AGB stars is a question which merits further studies. Note that Asplund et al. (1999) found the same figure in a post-AGB star and they concluded that they were observing the characteristic time scale of the mechanism responsible for the lithium production.

Qualitatively our NLTE results agree with RQ but quantitatively some discrepancies are found. For instance, inspection to their Fig. 7 shows a NLTE correction of  $\sim 0.7$  dex at  $\log \epsilon(\text{Li})=4$  for the  $\lambda 6708 \text{ \AA}$  line. However, our computations give a correction of  $\sim 0.4$  dex (see Fig. 2). This can be easily

explained by differences in the NLTE procedure, model atmospheres etc. *Namely*, in this paper we fully computed the opacities in the bound-free and bound-bound lithium transitions. This allowed us to establish the dependence of NLTE in lithium lines on C/O and the  $^{12}\text{C}/^{13}\text{C}$  isotopic ratio. Moreover, the analysis of RQ was based on the comparison between the LTE and NLTE curves of growths. Our LTE/NLTE spectral synthesis approach to determine Li abundances in the atmosphere of Li-rich AGB stars seems to be better. Only in this way is the lithium abundance determination possible, since the conventional definition of the equivalent width becomes meaningless due to the severe blending of Li lines. In this sense our results for subordinate Li lines are of great interest. Since we underestimate the opacity of the bound-free and bound-bound transitions of lithium we get an upper limit to the NLTE effects in these lines, but comparatively, we obtain low NLTE corrections on Li abundances. Using a more complete opacity source list, NLTE effects should be even less pronounced. That would comprise a good chance to obtain accurate abundance determinations based on the subordinate Li lines in the frame of the LTE approach, which is simpler and therefore more useful. On the other hand, we can only qualitatively compare our NLTE results with those by Pavlenko & Magazzú (1996) in M (O-rich) stars due to the obvious differences in opacities, model atmospheres etc, although in both cases, strong Li resonance lines are formed in the outermost layers of the atmosphere. Their curves of growth (see their Fig. 5) show a similar behaviour than ours (Figs. 1–2): for the  $\lambda 6708 \text{ \AA}$  line  $W_{\lambda}^{\text{LTE}} > W_{\lambda}^{\text{NLTE}}$  for  $\log \epsilon(\text{Li}) > 2$ ; i.e., in the case of strong lines formed high enough in the atmosphere NLTE effects reduce the equivalent width due to the dominant role of the overionization. For the  $\lambda 6104 \text{ \AA}$  Li line they found  $W_{\lambda}^{\text{LTE}} < W_{\lambda}^{\text{NLTE}}$  for  $\log \epsilon(\text{Li}) = 4.0$  (see their Fig. 6). However, we obtain the contrary. This can be explained since in our case (C-rich atmospheres) the overionization increase in the line-forming regions due to the lower density and pressure.

Abia et al. (1993a) computed an empirical Li yield from a homogeneous sample of galactic C-stars. They derived Li abundances from the  $\lambda 6708 \text{ \AA}$  line in  $\sim 220$  C-stars and by considering the mass-loss rate estimates for the stars in their study, obtained a Li yield into the interstellar medium of  $\sim 2 \times 10^{-9} M_{\odot} \text{ pc}^{-2} \text{ Gyr}^{-1}$ . These authors showed that this yield is extremely dependent on the stellar mass-loss rate assumed and on the real Li abundance in the star. Since approximately 90% of this value is determined by the actual yield from the SLiR C-stars, it is straightforward to revise this figure on the basis of the more accurate Li abundances obtained in this work. Now, considering the NLTE abundances obtained from the  $\lambda 8126 \text{ \AA}$  Li line as the best estimate of the lithium abundance, we obtain the revised yield of  $\sim 8 \times 10^{-10} M_{\odot} \text{ pc}^{-2} \text{ Gyr}^{-1}$ , a factor  $\sim 3$  lower than the previous value. This is mainly because the revised Li abundances in WX Cyg and IY Hya are considerably lower. As in Abia et al. (1993a), we can roughly estimate the contribution of C-stars to the galactic Li. Assume that the above production rate has been constant during the lifetime of the galaxy ( $\sim 13 \text{ Gyr}$ ) and that the surface density of C-stars has been uniform and also constant during this time within a galac-

tocentric radius of  $\sim 15 \text{ kpc}$  ( $\sim 50 \text{ C-stars kpc}^{-2}$ , see Clausen et al. 1987). In this case, the total contribution to galactic Li abundance by C-stars is  $M_{\text{Li}} \sim 3 M_{\odot}$ , i.e.  $\sim 10\%$  of the total Li in the galaxy. This contribution might be higher if evolutionary effects are taken into account, since the star formation rate was certainly higher in the past. Correspondingly, the number of C-stars that eventually became a SLiR C-star at a given time was also higher (see Abia et al. 1993a for details).

In summary:

1. The formation of the lithium resonance line in C-stars is severely affected by NLTE effects. NLTE Li abundances are higher and can differ from the LTE ones up to 0.6 dex. The core of this strong Li line is formed in the outermost layers where we approach the interstellar medium regime. Furthermore, these layers are affected by different phenomena such as the stellar chromosphere, inhomogeneities, dusty shells, outflow/infall velocities etc. Our computations also show that lithium is severely overionized. Therefore, the use of this saturated lithium line for abundance determinations in AGB stars seems quite impossible. In that sense, we confirm the results of RQ.
2. Subordinate lithium lines are formed in the inner parts of the atmosphere. We have shown that NLTE effects are rather weak even for strong lines (0.1–0.3 dex). Thus, they may be used for lithium abundance determinations in AGB stars even in the framework of the LTE approach. Of the three subordinate lines, the  $\lambda 8126 \text{ \AA}$  Li I line is probably the best one for Li abundance determinations because it is less blended, because NLTE effects are weak, because the molecular and atomic line list appears to be complete and because continuous opacity seems rather well reproduced in this spectral domain.
3. NLTE effects in the lithium lines show a complicated dependence on the input parameters  $T_{\text{eff}}$  and the C/O ratio. We found that NLTE effects increase with increasing  $T_{\text{eff}}$  and a decreasing C/O ratio. For a given  $T_{\text{eff}}$ , NLTE effects decrease with increasing Li abundance for the subordinate lines but increase for the resonance line. Furthermore, for high Li abundances ( $\log \epsilon(\text{Li}) > 4$ ) LTE/NLTE abundances from the subordinate lines are not very sensitive to  $T_{\text{eff}}$  or the C/O ratio. For the resonance line, however, the opposite happens.
4. The possibility of using the lithium subordinate doublet at  $\lambda 4603 \text{ \AA}$  was considered. Theoretical spectra, however, show a bad agreement with the observations, probably due to a wrong estimate of the continuous opacity in this spectral range and to an incomplete line list in this region. Furthermore, this lithium line forms a strong blend with iron lines. Due to the very weak NLTE corrections found for it, the use of this Li doublet would be promising in the case of metal deficient stars if using very high resolution spectra. Since we are confident of the atomic and molecular line list used beyond  $\sim 6000 \text{ \AA}$ , we suggest that the  $\text{C}_2$  lines of the Swan system observed in the blue part of the spectrum are the largest source of error. More accurate line lists for these transitions are therefore needed. Such an improvement, together with better atmosphere modelling, solving the problem of the missing continuous opacity in the blue part of

the spectrum, should improve the agreement between observed and synthetic spectra in the future.

5. We have used observational data of high quality to determine lithium abundances in three C-stars: WX Cyg, WZ Cas and IY Hya. We have shown, that they are indeed SLiR stars with Li abundances in the range  $\log \epsilon(\text{Li}) \approx 3$  to 5. However, up to now we have still failed to accurately determine Li abundances in AGB stars, mainly due to uncertainties in modelling their atmosphere. This leads to an important uncertainty concerning the estimate of the Li yield by AGB stars. These stars might account for up to 30% of the currently observed Li or merely be a secondary source of Li in the galaxy.

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