Statistical Equilibrium of Lithium in the Atmospheres of Late-Type Stars: Lithium-Rich G–K Giants

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Abstract—The calculations of statistical equilibrium of lithium in the atmospheres of G–K giants are discussed. The studies are carried out for a 20-level model of the Li atom by the complete-linearization method. Allowance is made for the blanketing effect produced by atomic, ionic, and molecular absorption. The dependence of the parameters of Li absorption lines on the model-atmosphere parameters log g and [Fe/H] is analyzed. It is shown that: (i) the non-LTE effects in Li lines differ markedly for specific K giants; the abundance correction due to these effects varies over a wide range: from ~0.4 dex (for HD 112127) to +0.2 dex (for Capella B); (ii) for K giants with $T_{\text{eff}} < 4500$ K, the non-LTE equivalent widths of saturated absorption lines are less sensitive to log g and [Fe/H] than their LTE values; and (iii) the solutions of the non-LTE problem for 6-level and 20-level model atoms are very close. For several giants, the lithium abundance has been redetermined by taking into account the departures from LTE.

INTRODUCTION

Lithium lines are of considerable interest in studies of the evolutionary status of G–K giants (Brown et al. 1989; Boyarchuk et al. 1991; Pilachowski and Sowell 1992). The Li abundance in the atmospheres of late-type stars has been mainly determined in the approximation of local thermodynamic equilibrium (LTE). At the same time, one should take into account the fact that Li lines can be significantly affected by departures from LTE (non-LTE effects). Indeed, lithium has a low ionization potential (5.3 eV), and its resonance lines ($\lambda$ 670.8 nm) of low excitation ($E_{\text{ex}} = 1.8$ eV) are, by the definition of Thomas (1957), governed by photoionization.

An analysis of departures from LTE in the Li lines that form in the atmospheres of G–K giants has been the subject of several studies (Pavlenko 1989, 1991a, 1991b, 1992; Luck 1977; Steenbock and Holweger 1984; Carlsson et al. 1994). The latter authors restricted their analysis to stars with $T_{\text{eff}} \geq 4500$ K.

In this paper, we perform the calculations for several lithium-rich K giants from the sample of Brown et al. (1989), for components A and B of the binary system Capella, which were studied by Pilachowski and Sowell (1992), and for 9 Boo (Khynni 1984). We model the Li lines in the spectrum of the latter star in the LTE approximation (Yakovina 1986) and by taking into account the departures from LTE (Pavlenko 1989). In the latter case, the calculations of a self-consistent system of statistical-balance and radiative-transfer equations (the non-LTE problem) are performed for simplified models of the Li atom and for a limited list of molecular opacity sources. The reliability of these results must be confirmed by further computations.

Thus, the prime objective of this study is to model the statistical equilibrium of lithium in the atmospheres of late-type giants by abandoning LTE. We use these computations to refine the abundance of lithium in the atmospheres of specific G–K giants by allowing for the non-LTE effects in its lines.

IONIZATION–DISSOCIATION EQUILIBRIUM

We calculated the chemical equilibrium in the atmospheres of red giants for 86 molecules and 36 atoms and their first ions (including lithium-containing molecules: LiO, LiH, LiBr, LiF, LiL, Li2, and LiOH) in the LTE approximation. The data for computing the dissociation equilibrium were taken from Tsuji (1973).

The Set of Opacity Sources

A major difficulty involved in computing model atmospheres and in solving non-LTE problems is the calculation of opacity in stellar atmospheres. Our method of calculating the opacity in the atmospheres of red giants, which is attributable to atomic and ionic absorption, is similar to the method described in Pavlenko (1994). When computing model atmospheres with $T_{\text{eff}} < 4500$ K, we allowed for the molecular absorption by the bands of 21 diatomic molecules in the JOLA (just overlapping line approximation) approximation using the BIGF code of A. Yaremchuk (Nersisyan et al. 1989). The JOLA approximation yields good results when computing saturated molecular bands. For weak molecular bands, the results are not so good (see Tsuji 1994), but for $T_{\text{eff}} > 4500$ K, the blanketing effect due to atomic and ionic absorption, which is taken into...
account by the opacity sampling method (Pavlenko and Yakovina 1994), is decisive.

Our list of molecular opacity sources is intended for computing absorption in the atmospheres of oxygen-sequenace stars, i.e., those with O/C > 1. We took into account the absorption by diatomic molecules alone. The data for these molecules are given in Pavlenko et al. (1995). Our experience of working with this set of molecular opacity sources shows that it describes fairly well the energy distribution in the visible spectral region of late M stars, in which the molecular absorption dominates.

The results of our calculations of the emergent flux from the atmosphere of 9 Boo (4200/1.5) for various opacity sources are shown in Fig. 1. As was noted in our previous paper (Pavlenko 1991a), the ionization equilibrium for lithium is mainly determined by the relationship between the photoionization from the second 2p level (\( \lambda_{\text{ion}} = 3500 \) Å) and the photorecombination to this level. In the atmospheres of G–K giants, the absorption by atomic lines dominates at the frequencies of bound-free 2p-continuum transitions in the Li atom (Fig. 1).

**STELLAR MODEL ATMOSPHERES**

We computed model atmospheres for the giants in the table using the SAM72 code. This is a version of the ATLAS9 code of Kurucz (1993a). The XLINOPOS subroutine, which allows for atomic and ionic absorption by the opacity sampling method, was taken from the SAM91 code (Pavlenko 1991c). We allowed for the molecular absorption by 21 diatomic molecules in the JOLA approximation. The stellar model atmospheres were computed by taking into account convection with the mixing scale length \( f_H = 1.25 \); the convective overshooting was ignored. The chemical composition of the model atmospheres was taken from Brown et al. (1989), Boyarchuk et al. (1991), and Pilachowski and Sowell (1992).

We tested the method of computing model atmospheres by comparing the temperature structures of the model atmospheres computed for a 3500/2.00 giant by us and by Kurucz (1993a). Despite the differences in the methods of allowance for the blanketing effect, good agreement with Kurucz's model was obtained. The temperature differences did not exceed 50 K almost over the entire depth of the model atmosphere (Pavlenko and Yakovina 1994).

1 In this paper, we use the notation A/B/C, where A, B, and C give the effective temperature \( T_{\text{eff}} \), gravity \( \log g \), and metallicity \( [\text{Fe/H}] = \log N(\text{Fe})_a - \log N(\text{Fe})_\odot \), respectively, for model atmospheres of specific stars. For 9 Boo, however, we use the abundances of several elements that were determined by Boyarchuk et al. (1991). Therefore, in this case (and in what follows), the third parameter (metallicity) in the designation of the model atmosphere for 9 Boo is omitted.

**The Method of Solving the Non-LTE Problem**

We used the complete-linearization method (Auer and Heasley 1976) to solve the system of equations of the non-LTE problem. The principal features of this method are listed below:

1) The non-LTE problem was solved for a 20-level Li model atom described in Pavlenko (1994). Each Li multiplet was replaced by a single line, a standard procedure in such calculations (see Steenbock and Holweger 1984). The absorption-coefficient profile of Li lines allowed us to take their multiplet structure into account (Pavlenko 1989).

2) We calculated the rates of transitions produced by inelastic collisions with electrons using the formulas from Pavlenko (1984).

3) In our previous papers (Pavlenko 1989, 1991a, 1991b), we also took into account the transitions between Li levels produced by collisions of the second kind with hydrogen atoms. However, more recent studies (Lambert 1993) have shown that the formulas of Steenbock and Holweger (1984) yield highly overestimated values of the corresponding rates of transitions between Li levels. Therefore, we ignored the excitation and deexcitation of the Li atom by inelastic collisions with hydrogen atoms (see also Carlson et al. 1994).

4) We solved the non-LTE problem for lithium in the approximation of an admixed element, i.e., we assumed that changes in its ionization equilibrium could not affect the structure of the stellar model atmosphere. This assumption holds in the atmospheres of stars with \( T_{\text{eff}} > 2500 \) K (Pavlenko et al. 1995).
Atmospheric parameters of K giants and the Li abundances in their atmospheres

<table>
<thead>
<tr>
<th>Star</th>
<th>$T_{\text{eff}}$</th>
<th>log $g$</th>
<th>[Fe/H]</th>
<th>log N(Li) LTE</th>
<th>log N(Li) non-LTE</th>
<th>Correction D</th>
<th>previous estimates</th>
</tr>
</thead>
<tbody>
<tr>
<td>HD 787</td>
<td>4220</td>
<td>1.5</td>
<td>0.07$^{1)}$</td>
<td>1.8</td>
<td>1.71</td>
<td>-0.09</td>
<td></td>
</tr>
<tr>
<td>HD 9746</td>
<td>4420</td>
<td>2.3</td>
<td>-0.13$^{1)}$</td>
<td>2.7</td>
<td>2.40</td>
<td>-0.30</td>
<td>-0.30$^{5)}$</td>
</tr>
<tr>
<td>HD 30834</td>
<td>4190</td>
<td>1.5</td>
<td>-0.17$^{1)}$</td>
<td>1.8</td>
<td>1.73</td>
<td>-0.07</td>
<td></td>
</tr>
<tr>
<td>HD 10847</td>
<td>4970</td>
<td>2.8</td>
<td>-0.02$^{1)}$</td>
<td>2.0</td>
<td>2.07</td>
<td>0.07</td>
<td></td>
</tr>
<tr>
<td>HD 112127</td>
<td>4340</td>
<td>2.1</td>
<td>+0.31$^{1)}$</td>
<td>2.7</td>
<td>2.30</td>
<td>-0.40</td>
<td>-0.40$^{5)}$</td>
</tr>
<tr>
<td>HD 120602</td>
<td>5000</td>
<td>3.0</td>
<td>-0.07$^{1)}$</td>
<td>1.9</td>
<td>1.98</td>
<td>0.08</td>
<td></td>
</tr>
<tr>
<td>HD 126868</td>
<td>5440</td>
<td>3.2</td>
<td>-0.25$^{1)}$</td>
<td>2.3</td>
<td>2.34</td>
<td>0.04</td>
<td></td>
</tr>
<tr>
<td>HD 148293</td>
<td>4640</td>
<td>2.5</td>
<td>+0.23$^{1)}$</td>
<td>2.1</td>
<td>2.14</td>
<td>0.14</td>
<td></td>
</tr>
<tr>
<td>HD 183492</td>
<td>4700</td>
<td>2.4</td>
<td>+0.08$^{1)}$</td>
<td>2.0</td>
<td>2.15</td>
<td>0.15</td>
<td></td>
</tr>
<tr>
<td>HD 205349</td>
<td>4480</td>
<td>0.6</td>
<td>0$^{2)}$</td>
<td>1.9</td>
<td>1.89</td>
<td>-0.01</td>
<td></td>
</tr>
<tr>
<td>Capella A</td>
<td>4800</td>
<td>2.6</td>
<td>0$^{2)}$</td>
<td>0.86</td>
<td>1.03</td>
<td>0.17</td>
<td></td>
</tr>
<tr>
<td>Capella B</td>
<td>5550</td>
<td>2.9</td>
<td>0$^{2)}$</td>
<td>3.10</td>
<td>2.94</td>
<td>-0.16</td>
<td></td>
</tr>
<tr>
<td>9 Boo</td>
<td>4200</td>
<td>1.0</td>
<td>0$^{3)}$</td>
<td>2.00</td>
<td>2.10</td>
<td>0.10</td>
<td>0.15$^{6)}$</td>
</tr>
</tbody>
</table>

Note: $^{1)}$Brown et al. (1989); $^{2)}$Pilachowski and Sowell (1992); $^{3)}$Yakovina (1986); $^{4)}$Boyarchuk et al. (1991); $^{5)}$Pavlenko (1992); $^{6)}$Pavlenko (1989).

(5) The absorption by the lithium atoms themselves at the frequencies of most of its radiative transitions is insignificant. This makes it possible to compute the rates of such transitions in the approximation of fixed rates, which considerably simplifies the computational procedure. In our case, we applied the linearization procedure only to the ten strongest radiative transitions of lithium from the first (2s) and second (2p) excited states, which can form detectable absorption lines in the spectra of cool stars for reasonable abundances of this element.

(6) When solving the non-LTE problem, we allowed for atomic, ionic, and molecular absorption at the frequencies of bound-bound transitions in a straightforward way, as in the calculations of synthetic spectra.

(7) The rates of radiative bound-free transitions of lithium were computed in the approximation of fixed rates. The intensity of the radiation field at the corresponding frequencies was averaged over the 0.4-nm interval; we allowed for the entire set of opacity sources, including the opacity attributable to the absorption by lines of other atoms and ions (Pavlenko 1991b).

Note that our method of calculating the opacity takes into account the fact that the chemical composition of stellar atmospheres is unique. This seems especially important in the case of red giants, which normally have a chemical composition that differs from that of the Sun.

RESULTS

The fact that the nature of non-LTE effects in the Li lines that form in the atmospheres of G–K giants is essentially the same as that for stars of lower luminosities is currently believed to be an established fact. We also modeled Li lines in the spectra of G–K dwarfs and subgiants by abandoning LTE (see Pavlenko 1994; Pavlenko et al. 1995).

Menzel’s Coefficients

It is advantageous to use Menzel’s coefficients $b_i = n_i/n_i^s$, where $n_i^s$ and $n_i$ are the LTE and non-LTE populations of the $i$th level, respectively, to describe changes in the level populations of the Li atom. Figure 2 shows Menzel’s coefficients of the Li levels that we calculated for two Li abundances for a model atmosphere of 9 Boo (4200/1.5). In order not to overload the figure, only two lower and two upper levels of the adopted model atom are shown. Note that the second and eighteenth levels are coupled with the ground level of lithium (2s) by fairly strong radiative transitions.

For log N(Li) = 1.0, the Li resonance lines (the 2s–2p transition) are unsaturated. Menzel’s coefficients of the lower levels are smaller than unity; they increase with level number (see also Steenbock and Holweger 1984; Pavlenko 1994). The decrease in the population of the Li levels (compared to LTE) is attributable to the dominance of photionization over photorecombination (to the reionization of lithium).

For log N(Li) = 2.0, the Li lines are rather strong ($W_\lambda = 200$ μA); in a fairly wide interval of depths in the
stellar atmosphere, \( \tau \gg 1.0 \) at their frequencies. In this case, there is a balance of radiative transitions between the first and second levels, which leads to a weakening of the radiative coupling between these levels. Other chains of transitions to the first level from other levels (including those from the continuum), whose populations are increased compared to LTE, emerge. As a result, there is a sufficiently extended region, where \( b_1 > b_2 \), in which the interrelation between the transitions in the stellar atmosphere dominates.

Note that:

(i) as was pointed out above, the population of the second level of lithium is governed by photoionization, and they change only slightly as the Li abundance increases;

(ii) for large Li abundances \( \log N(\text{Li}) = 3.0 \) in the stellar atmosphere, the population of the first level of lithium can be even greater than the LTE values (Pavlenko 1992);

(iii) the upper levels that are not coupled with the lower levels by radiative transitions turn out to be more coupled with the continuum than with the lower-lying levels. In our case, \( b_{10} > 1.0 \) in a fairly wide interval of depths.

Thus, the term “lithium reionization” can only be used to describe the overionization of lithium (compared to LTE) and not to describe the distribution of its populations in excited states (see also Pavlenko and Magazzu 1996).

The Curves of Growth of Li Lines for 9 Boo

We computed the curves of growth of Li absorption lines in the LTE approximation and by abandoning LTE. In the latter case, we used the solution of a multilevel non-LTE problem. The profile of an individual line (or a component of a multiplet) was described by Voigt’s formula. In the calculations of the damping constant, we took into account natural damping and van der Waals and Stark broadening (Pavlenko and Shavrina 1986). The correction factor \( E = 1.5 \) (Andretta et al. 1991) was used to calculate \( \gamma_c \). We computed the curves of growth for the microturbulent velocity \( v_t = 2 \text{ km s}^{-1} \).

A comparison of the LTE and non-LTE curves of growth is of particular interest, because it allows us to determine the non-LTE correction to the Li abundance: \( \Delta = \log N_{\text{non-LTE}}(\text{Li}) - \log N_{\text{LTE}}(\text{Li}) \). Figure 3 shows the curves of growth of Li lines computed for the model atmosphere of 9 Boo. The ranges of positive and negative values of \( \Delta \) for the resonance doublet of lithium are denoted by A and B, respectively. In range A, \( \Delta > 0 \); here Li reionization dominates. In range B, \( \Delta < 0 \); the coupling of levels is more important (Pavlenko 1992; Carlsson et al. 1994). In our previous paper (Pavlenko 1989), by solving the non-LTE problem for a six-level model of the Li atom for the model atmosphere of 9 Boo, we found that \( \Delta = 0.1 \) dex. In this paper, by solving the non-LTE problem for a 20-level Li model atom, we obtained essentially the same value of \( \Delta \).

Recently, with the realization that several serious methodical problems (Dunkan 1991; Pavlenko and Magazzu 1996) must be solved for a quantitative analysis of strong saturated Li I lines, the interest to the study of its subordinate lines has increased. This prompted us to extend the scope of the study. In particular, below we perform the non-LTE calculations for the subordinate Li I lines at \( \lambda \lambda \) 812.6 and 610.3 nm. Note that the second line is more intense, but it lies in a more blended region of the spectrum. On the other hand, there is an extensive spectrum of telluric lines near \( \lambda \) 812.6 nm.

As follows from Fig. 3, \( \Delta > 0 \) for the subordinate Li I lines that form in the atmosphere of 9 Boo in a wide range of lithium abundances.

Figure 3 also shows the LTE and non-LTE curves of growth of the resonance Li I doublet computed for the model atmospheres of the star with the same value of \( T_{\text{eff}} \) but with different \( \log g \) and metallicities. In our opinion, an important result of this work is the demonstration that the non-LTE curves of growth at \( T_{\text{eff}} < 4500 \text{ K} \) are generally less sensitive to such stellar-atmosphere parameters as the luminosity and metallicity. This effect can be explained as follows: since the resonance Li I lines are governed by photoionization, their behavior largely depends on the radiation field that is formed at the level of the stellar photospheres. It turns out that at \( T_{\text{eff}} < 4500 \text{ K} \) the radiation field emerging from the photosphere depends rather weakly on \( \log g \) and metallicity, because at the level \( \tau \approx 1 \) the electron number densities in these model atmospheres differ.

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Aside from a purely academic interest, the results described above are important in refining the evolutionary status of the above stars. For example, the unification of HD 9746, HD 112127, and 9 Boo into a single group of stars (see Berdyugina and Savanov 1994) seems more justified by using the non-LTE computations of the Li abundance,

$$\log N_{\text{non-LTE}}(\text{Li}) = 2.4, 2.3, 2.1.$$  

Let us compare these Li-abundance determinations with the LTE values

$$\log N_{\text{LTE}}(\text{Li}) = 2.7, 27, 2.0.$$  

Among other results, note also good agreement of the new data for 9 Boo, HD 9746, and HD 112127 with the results of Pavlenko (1989, 1992), in which the non-LTE problems were solved for a six-level Li model atom.

**DISCUSSION OF THE RESULTS**

It should be noted that there is general agreement between the researchers concerning the magnitude and role of the non-LTE effects in forming the Li lines in stellar atmospheres. For example, a comparison of our non-LTE corrections to the Li abundance (Pavlenko 1994; Pavlenko and Magazzu 1996) with the data of Carlsson et al. (1994) for F–G stars indicates that the differences between them do not exceed 0.1 dex for strong lines. For weak lines, the agreement between the non-LTE calculations is even better (Pavlenko and Magazzu 1996). Note that these differences are determined by the cumulative effect of the differences in the model atoms, model atmospheres, and cross sections. In this case, they are also definitely smaller than the absolute non-LTE corrections to the Li abundance.

For several red giants, Luck (1977) obtained considerably larger non-LTE corrections than our values. Clearly, this can be explained by the fact that Luck took into account only the continuum absorption at the frequencies of bound-free transitions of lithium. In this case, the calculations of blanketing in the violet and in the ultraviolet yield overestimated theoretical fluxes (Fig. 1). As a result, the reionization processes are artificially enhanced, and the non-LTE abundance corrections sharply increase (see Steenbock and Holweger 1984).

As was pointed out above (when describing the method of calculations), we ignored the transitions between the Li atomic levels produced by inelastic collisions with hydrogen atoms. Note that their formal inclusion in the rate matrix of the corresponding transitions calculated from the formulas of Steenbock and Holweger (1984) leads to a systematic shift of the non-LTE curves of growth toward larger values of $W_{\lambda}$ and, consequently, to a change of $\Delta$. The absolute value of $\Delta$ decreased for weak lines and increased for strong lines. In any case, these changes turned out to be small. For example, we obtained $\log N(\text{Li})_{\text{Ch}}^{\text{non-LTE}} = 0.98$ for

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**Redetermination of the Li Abundance with Allowance for Departures from LTE**

The Li abundances in the atmospheres of several G–K giants that we determined by taking into account the departures from LTE are given in the table. We performed the non-LTE calculations using the scheme that was described above for 9 Boo; it involved the computation of a model atmosphere of specified chemical composition, the solution of the non-LTE problem, the computation of the LTE and non-LTE curves of growth, and the redetermination of $\log N(\text{Li})$.

As can be seen from the table, the non-LTE corrections are small ($\Delta \approx 0.1$ dex) for a sizable fraction of the giants. However, this factor suggests not so much a low efficiency of the non-LTE effects in the atmospheres of these stars as the balance of reionization processes and the coupling of transitions, which are capable of canceling each other.
Capella A and \( \log N(\text{Li})_{\text{non-LTE}} \) = 2.93 for Capella B (cf. the table). However, these results can also be interpreted as evidence that the solution of the non-LTE problem for lithium is virtually insensitive to the collision rates.

This solution depends to a greater extent on the radiation field at the frequencies of radiative transitions of lithium. Therefore, the reliability of this kind of results is severely limited by incompleteness of the list of opacity sources, whose nomenclature is significantly extended as the effective temperature of the star decreases. With the publication of new lists by Kurucz (1992, 1994), considerable progress has been made in solving this problem. At the same time, these lists are also far from being complete. In this sense, the JOLA approximation for computing molecular opacity currently remains important, especially since our list of molecular bands that we took into account surpasses the list of Kurucz (1993b) in completeness. Note that the frequencies of bound-free transitions of lithium lie in a relatively long-wavelength part of the spectrum, in which the information on molecular absorption is fuller and more accurate.

The stars in the table differ in evolutionary status. Among them there are giants of the first ascent (HD 787, HD 9746, 9 Boo) and giants in the stage of core-helium burning (HD 30834, HD 120602) (Brown et al. 1989; Boyarchuk et al. 1991; Berdyugina and Savanov 1994). In general, giants of different ages differ by the activity in their atmospheres. Some of these stars definitely have chromospheres of different strengths. This problem is particularly important for Capella B; it belongs to the class of RS CVn stars (Savanov 1990), which are characterized by strong chromospheric activity. The influence of the chromospheres on the Li lines that form in the atmospheres of G–K giants is beyond the scope of this paper. Note, however, that our previous studies (Pavlenko et al. 1995) have shown that the Li lines in late-type dwarfs and subgiants hardly “feel” a chromosphere comparable in strength to the solar chromosphere. This is because, the Li lines, as was pointed out above, are governed by photoionization, i.e., they depend to a greater extent on the radiation field that forms in the photospheric levels. Only stronger chromospheres which produce the veiling effect can significantly affect the intensities of Li absorption lines (see also Houdébine and Doyle 1995). This problem for red giants will be considered in more detail in a separate paper.

As part of this work, we carried out our studies for homogeneous model atmospheres. The photospheres of red giants lie at the upper boundary of their convective envelopes. Since the granules in such envelopes are fairly large, the horizontal atmospheric inhomogeneity increases. This inhomogeneity must also be taken into account in a more detailed analysis. In our opinion, this factor has a greater effect on the lines of atoms and ions that are governed by collisions.

CONCLUSION

Thus, the non-LTE effects for saturated Li lines in the spectra of red giants are clearly systematic in nature: allowance for the non-LTE effects in such lines reduces the lithium abundance. Consequently, the Li lines in the spectra of late-type giants must be modeled and interpreted by taking into account the non-LTE effects.

Another important result of this study is the demonstration that the Li lines which we computed by taking into account departures from LTE are less sensitive to such important but often poorly determined, stellar parameters as the luminosity and metallicity. In this sense, non-LTE calculations yield more reliable estimates of the lithium abundance in stellar atmospheres.

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REFERENCES


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