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On the lithium abundance of the visual binary components \( \xi \) Boo A (G8V) and \( \xi \) Boo B (K5V)

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Abstract

A spectroscopic investigation of the lithium resonance doublet in \( \xi \) Boo A and \( \xi \) Boo B in terms of both abundance and isotopic ratio is presented. We obtained new \( R=130\,000 \) spectra with a signal-to-noise ratio (S/N) per pixel of up to 3200 using the 11.8m LBT and PEPSI. From fits with synthetic line profiles based on 1D-LTE MARCS model atmospheres and 3D-NLTE corrections, we determine the abundances of both isotopes. For \( \xi \) Boo A, we find \( A(\text{Li}) = 2.40 \pm 0.03 \) dex and \( ^6\text{Li}/^7\text{Li} < 1.5 \pm 1.0 \% \) in 1D-LTE, which increases to \( \approx 2.45 \) for the 3D-NLTE case. For \( \xi \) Boo B we obtain \( A(\text{Li}) = 0.37 \pm 0.09 \) dex in 1D-LTE with an unspecified \( ^6\text{Li}/^7\text{Li} \) level. Therefore, no \( ^6\text{Li} \) is seen on any of the two stars. We consider a spot model for the Li fit for \( \xi \) Boo B and find \( A(\text{Li}) = 0.45 \pm 0.09 \) dex. The \( ^7\text{Li} \) abundance is 23 times higher for \( \xi \) Boo A than the Sun's, but three times lower than the Sun's for \( \xi \) Boo B while both fit the trend of single stars in the similar-aged M35 open cluster. Effective temperatures are redetermined from the TiO band head strength. We note that the best-fit global metallicities are \( -0.13 \pm 0.01 \) dex for \( \xi \) Boo A but \( +0.13 \pm 0.02 \) dex for \( \xi \) Boo B. Lithium abundance for the K5V benchmark star 61 Cyg A was obtained to \( A(\text{Li}) \approx 0.53 \) dex when including a spot model but to \( \approx 0.15 \) dex without a spot model.

KEYWORDS:
stars: abundances, stars: activity, stars: binaries: visual, stars: atmospheres, stars: spots

1 | INTRODUCTION

\( \xi \) Boo (HIP 72659, GJ566) is a nearby visual binary with two bright components denoted as \( \xi \) Boo A (HD 131156A) and \( \xi \) Boo B (HD 131156B). The AB orbital period is 151 yr in a strongly inclined 0.51-eccentricity orbit (Wielen 1962). Its inclination of 140\( ^\circ \) means retrograde motion with respect to increasing position angles and a residual inclination with respect to the plane of the sky of 50\( ^\circ \). The current apparent AB separation is 7.15\". The A primary component is a solar-like star of spectral type around G8V while the B secondary component is a significantly cooler and lower mass star of spectral type K4-5V (Abt 1981, Levato & Abt 1978). Both components have moderately strong and variable Ca II emission (Wilson 1978) with irregular long-term fluctuations (Lockwood et al. 2007, Baliunas et al. 1995). Its strengths indicate surface magnetic activity exceeding that of the Sun by about a factor 2–3. Due to its brightness the system had been the target of numerous observations ranging from X-rays (e.g., Johnstone & Güdel 2015; Wood et al. 2018) to radio wavelengths (e.g., Linsky & Gary 1983 and references therein).

Of most interest in the context of the present paper is the fact that the A component shows strong Li I 6708-Å absorption while the B component has an essentially undetected Li I 6708-Å line. This was already noticed by Wilson (1963) and Herbig (1965), and confirmed by Savanov (1992). The absent Li in the B component had been attributed to the expected

Abbreviations:
PEPSI Potsdam Echelle Polarimetric and Spectroscopic Instrument. LBT Large Binocular Telescope. (N)LTE (Non)Local Thermodynamic Equilibrium.
strong convective mixing and thermonuclear destruction of Li in such a very cool star. The presence of strong Li in the G8V component with an abundance of $\text{A(Li)} \approx 2.4$ (Luck 2017) is a sign of youth, or the lack of above mentioned convective mixing. It appears not an uncommon value among late-to-mid G stars only slightly older than the Pleiades for which Bouvier et al. (2018) quote abundances of $\approx 2.7$ for temperatures around 5500 K, but noticed and emphasized the large spread of 0.5–2.5 for the cooler temperatures around $\approx 4600$ K.

Standard stellar evolution models predict already significant lithium depletion during the pre-main sequence phase, whereas they wrongly predict little or no depletion during the main sequence (e.g., Iben 1965). Therefore, the standard models overestimate the present-day solar lithium abundance by about a factor of 100, and thus are also at odds with the depletion pattern observed in open clusters (e.g., Iben 1965). Therefore, the standard models overestimate the present-day solar lithium abundance by about a factor of 100, and thus are also at odds with the depletion pattern observed in open clusters (e.g., Iben 1965). Therefore, the standard models overestimate the present-day solar lithium abundance by about a factor of 100, and thus are also at odds with the depletion pattern observed in open clusters (e.g., Iben 1965). Therefore, the standard models overestimate the present-day solar lithium abundance by about a factor of 100, and thus are also at odds with the depletion pattern observed in open clusters (e.g., Iben 1965). Therefore, the standard models overestimate the present-day solar lithium abundance by about a factor of 100, and thus are also at odds with the depletion pattern observed in open clusters (e.g., Iben 1965). Therefore, the standard models overestimate the present-day solar lithium abundance by about a factor of 100, and thus are also at odds with the depletion pattern observed in open clusters (e.g., Iben 1965). Therefore, the standard models overestimate the present-day solar lithium abundance by about a factor of 100.

Section 2 describes our new observations. Section 3 is a review of the stellar parameters of $\zeta$ Boo. Section 4 is the analysis for the two stars including 61 Cyg A for comparison, and Section 5 a brief summary and conclusion. In the Appendix, we address the question whether star spots are the cause of enhanced TiO line strength and present a numerical study of TiO line strengths as a function of stellar effective temperature, star spot temperature and area filling factor.

2 OBSERVATIONS

New high-resolution, high S/N spectra were obtained with PEPSI (Strassmeier et al. 2015) at the effective 11.8 m LBT (Hill et al. 2012) in southern Arizona. The two 8.4 m LBT mirrors (dubbed SX and DX) were used in binocular mode, that is like a single 11.8 m telescope, which for PEPSI is achieved by combining the spectra from the two mirrors after integration. For the current observations PEPSI itself was fed through its IQUV polarimeters at the two straight-through Gregorian foci. For Stokes I all six individual QUV exposures

\[ \text{A(Li)} = \log(N_{\text{Li}}/N_{\text{H}}) + 12 \]
TABLE 1 Adopted astrophysical properties of \( \xi \) Boo A and \( \xi \) Boo B.

| Parameter                  | \( \xi \) Boo A | Ref. | \( \xi \) Boo B | Ref. |
|----------------------------|----------------|------|----------------|------|
| Classification, MK         | G8V            | (1)  | K5V            | (1)  |
| Effective temperature, K   | 5480           | (9)  | 4570           | this paper |
| Log gravity, cm s\(^{-2}\) | 4.53           | (9)  | 5.0            | (9)  |
| \( v \sin i \), km s\(^{-1}\) | 3.0            | (2)  | 1.5            | this paper |
| Microturbulence, km s\(^{-1}\) | 1.40         | (9)  | 0.15           | (9)  |
| Macroturbulence, km s\(^{-1}\) | 3.6            | (3)  | ...            |      |
| Rotation period, d         | 6.43           | (6)  | 11.94          | (8)  |
| Inclination, deg           | 28±5           | (5,11) | ≈32         | this paper |
| Iron abundance, H=12       | 7.29           | (9)  | 7.45           | (9)  |
| Distance, pc               | 6.753          | (10) | 6.748          | (10) |
| Luminosity, \( L_\odot \)  | 0.55           | (9)  | 0.17           | this paper |
| Radius, \( R_\odot \)      | 0.82           | (9,10) | 0.66         | assumed |
| Age, Myr                   | 187            | (12) | 265            | (12) |

(1) Abt (1981). (2) Gray (1994). (3) Allende Prieto et al. 2004. (4) Fernandes et al. (1998). (5) Petit et al. (2005). (6) Toner & Gray (1988). (7) Ruck & Smith (1995). (8) Donahue et al. (1996). (9) Luck (2017). (10) Gaia DR-3 (2022). (11) Morgenthaler et al. (2012). (12) Barnes (2007).

were combined for its final spectrum according to a total exposure time of 30 min for \( \xi \) Boo A and 60 min for \( \xi \) Boo B. The two pairs of 200 \( \mu \)m fibers result in a spectral resolution of \( R = \lambda / \Delta \lambda = 130,000 \) sampled by 4.2 pixels.

Observations of both \( \xi \) Boo components were spread over 10 consecutive nights in May 6-16, 2019. Eight and six individual spectra for \( \xi \) Boo A and \( \xi \) Boo B respectively, were obtained with cross disperser (CD) III covering 4800–5441 Å and with CD V covering 6278–7419 Å, the latter contains the lithium line at 6708 Å. Six individual exposures with an exposure time of 5 min for \( \xi \) Boo A and 10 min for \( \xi \) Boo B make up one phase spectrum. It resulted in S/N per pixel of up to 3200 in CD V with an average of 2,670 at the location of the lithium line for \( \xi \) Boo A, and up to 1700 for \( \xi \) Boo B with an average of 1450 at 6708 Å. Note that one spectrum of \( \xi \) Boo B was taken during bad weather conditions and reached S/N of just 215. Fig. 1 shows example spectra for both stellar components. The log of all observations is given in the Appendix in Table B3.

Data reduction was performed semi-automatically with the software package SDS4PEPSI (Spectroscopic Data Systems for PEPSI) based on the original code of Ilyin (2000), and described in some detail in Strassmeier et al. (2015, 2018a). The specific steps of image processing include bias subtraction and variance estimation of the source images, super-master flat field correction for the CCD spatial noise, scattered light subtraction, definition of échelle orders, wavelength solution for the ThAr images, optimal extraction of image slicers and cosmic spikes elimination, normalization to the master flat field spectrum to remove CCD fringes and the blaze function, a global 2D fit to the continuum, and the rectification of all spectral orders into a 1D spectrum.

3 REVIEW OF RELEVANT \( \xi \) BOO A AND \( \xi \) BOO B DATA

Table [1] summarizes the stellar input parameters for both components for our lithium fit. \( \xi \) Boo A’s fundamental stellar parameters were collected and discussed in Petit et al. (2005). This paper serves as the basis for our updated and extended summary. Note that a total of 29 papers are listed in CDS/Simbad for \( \xi \) Boo A which present a determination of effective temperature \( T_{\text{eff}} \), gravity \( \log g \), and/or metallicity \([\text{M/H}]\) or relative iron abundance \([\text{Fe/H}]\). A mean effective temperature of 5550 K for \( \xi \) Boo A was obtained by Gray (1994) from spectral line ratios. Savanov (1992) applied a model-atmosphere analysis to their high-dispersion photographic spectra and obtained effective temperatures for A and B of 5300±100 K and ≈4300 K, and gravities of 4.1±0.2 and ≈4.5, respectively. The metallicity of the primary was initially given as −0.20±0.08 by Cayrel de Strobel et al. (1992). Ruck & Smith (1995) presented a fine analysis of calcium and iron lines from \( R = 100,000 \) spectra of \( \xi \) Boo A and found 5500±70 K,
log g = 4.6 ± 0.1, and relative abundances of [Fe/H] and [Ca/H] of −0.15 and −0.13, respectively, with typical errors of ±0.05. The S4N catalog (Allende Prieto et al. 2004) lists component A with $3530 ± 115$ K, gravity of $4.576 ± 0.050$, and an absolute abundance [Fe/H] = 7.33, obtained with a microturbulence of $1.19 \text{ km s}^{-1}$ and a (Gaussian) macroturbulence of $3.64 \text{ km s}^{-1}$. The analysis in the catalog of Luck (2017) provides probably the most consistent stellar parameters. They list $\xi$ Boo A with $T_{\text{eff}} = 5480 \pm 33$ K, log $g = 4.53$, with a microturbulence of $1.38 \text{ km s}^{-1}$, a $\sin i$ of $6.0 \text{ km s}^{-1}$, and an absolute [Fe/H] abundance of $7.29 \pm 0.05$. No macroturbulence is stated though, which may explain the discrepancy in $\sin i$ to other measurements, for example those from Gray (1994) or Toner & LaBonte (1991) of $\approx 3 \text{ km s}^{-1}$.

For component B, Luck (2017) derived $T_{\text{eff}}$ of $4767$ K, log $g$ of 5.0, with a microturbulence of $0.15 \text{ km s}^{-1}$, a $\sin i$ of $5.1 \text{ km s}^{-1}$, and an absolute [Fe/H] abundance of $7.45 \pm 0.15$ (no other errors given). Our spectra show that Hα and Hβ appear as wingless but otherwise strong absorption lines. The rotational line broadening is a factor two smaller for $\xi$ Boo B than for $\xi$ Boo A, in particular for temperature and gravity insensitive lines, while line equivalent widths for $\xi$ Boo B can be larger by a factor 2–3 for gravity-sensitive lines compared to $\xi$ Boo A. This may have been reflected in the $\xi$ Boo B analysis of Luck (2017) by their comparably small microturbulence broadening of $0.15 \text{ km s}^{-1}$ combined with a too large $\sin i$ of $5.1 \text{ km s}^{-1}$. Takeda et al. (2007) used spectra from the Keck-based SPOCS catalog (Valenti & Fischer 2005) to also obtain absolute parameters for both components. While their results for $\xi$ Boo A ($T_{\text{eff}} = 5570 \pm 31$ K, log $g = 4.57 \pm 0.02$, [Fe/H] = $-0.07 \pm 0.02$) are consistent with other determinations, their values for $\xi$ Boo B have a lower gravity ($4.40$) and thus a higher mass ($0.99 M_\odot$) than for component A ($0.93 M_\odot$), and thus appear to be grossly inconsistent with the component’s apparent brightness. The Gaia DR-3 parallaxes of both components are practically identical ($6.753 \pm 0.006$ pc for A and $6.748 \pm 0.002$ for B) and, together with the fact that they form a physically connected binary, makes them likely also coeval. We also note that the DR3-based Apsis FLAME luminosity and radii for both components (A: $0.55 \pm 0.01$ $L_\odot$, $0.86 \pm 0.02$ $R_\odot$; B: $0.13 \pm 0.01$ $L_\odot$, $0.66 \pm 0.02$ $R_\odot$) agree very well with our values in Table 1.

Age determinations for the two components are unsurprisingly widespread. Most of the values come from comparisons of the spectroscopically determined fundamental parameters with evolutionary tracks and their isochrones. Fernandez et al. (1998) were among the first with a consistent modern analysis that led them to ages of $2 \pm 2$ Gyr, already indicating the complexity of the data situation. Takeda et al. (2007) compared their SPOCS-based stellar parameters with YREC tracks and derived the rather inconsistent ages of $<0.76$ Gyr for $\xi$ Boo A and 12.60 Gyr for $\xi$ Boo B. Based on Ca II H&K emission and a common age-activity relation, Wright et al. (2004) obtained ages of $0.00 – 0.35$ Gyr for A and $0.18 – 3.89$ Gyr for B. The measured rotation periods of A and B of 6.4 and 11.9 d, together with mean $B – V$’s of 0.76 mag and 1.17 mag for the two components, respectively, led Barnes (2007) to a 187 Myr based gyrochronological age for component A and 265 Myr for component B. Given the inherent uncertainties in gyrochronology, these ages are likely consistent with each other. No asteroseismic ages for either component are available to date.

## 4 ANALYSIS

### 4.1 Model atmospheres and spectrum synthesis

We basically follow our previous Li analysis in Mott et al. (2017) updated by the results from the detailed 3D non-LTE vs. 1D LTE comparisons in Mott et al. (2020) and Harutyunyan et al. (2018). Therefore, in the present paper, we only synthesize 1D LTE spectra for the astrophysical parameters of $\xi$ Boo A and $\xi$ Boo B and then apply 3D non-LTE corrections if available from previous calibrations. The Turbospectrum package (Plez 2012) is employed under the assumption of LTE to create the synthetic spectra.

The model atmospheres we used are those from MARCS (Gustafsson et al. 2008). A sample of atmospheres is chosen such that they bracket the stellar parameters listed in Table 1. A total of 400 spectra are synthesized per model atmosphere covering 20 Li abundances and five isotope ratios (each for four values for the microturbulence) and thus cover a 6-dimensional parameter space including $T_{\text{eff}}$, log $g$, [Fe/H], and microturbulence $\xi_{\text{micro}}$. The latter is not used as a free parameter in the line fit but was fixed to the values given in Table 1. Note that it describes a depth-independent isotropic Gaussian velocity distribution with a dispersion of $v_{\text{rms}} = \xi_{\text{micro}}/\sqrt{2}$.

### 4.2 Line list

Based on the four line-list comparisons in a previous application by Mott et al. (2017), we favor the line list collected by Meléndez et al. (2012) expanded by the vanadium revision of Lawler et al. (2014). Lawler et al. (2014) provided improved values of both wavelength and oscillator strength for the V1 blend close to one of the $^6$Li components ($\lambda = 6708.1096$ Å, log $gf = -2.63$). We use these values for V1 6708.094 Å instead of the ones in Meléndez et al. (2012). Apart from lithium, the total number of lines in this list is 36. The wavelengths are indicated as short vertical dashes in Fig. 1.
The four lithium transitions are implemented with their hyperfine structure (HFS) with a total of 12 line components and are based on Kurucz (2006). For each isotope separately, we add up the hyperfine fractional strengths of transitions between the same fine structure levels (characterized by quantum number $J$) but different hyperfine levels (characterized by quantum number $F$) that have (nearly) identical wavelengths. In this way, ten transitions of $^7\text{Li}$ can be reduced to six, and nine transitions of $^6\text{Li}$ can also be reduced to six, resulting in the 12-component representation of the isotopic HFS of the lithium resonance doublet given originally in Mott et al. (2017). The main differences between Kurucz (1995), his Table 1, and Kurucz (2006) are slight wavelength shifts of the HFS components of up to 2 mÅ for $^6\text{Li}$ and up to 8 mÅ for $^7\text{Li}$. Wavelength uncertainties of this order are considered irrelevant since such changes in the wavelength shifts are a factor 20 smaller than the separation of the fine structure doublet components of each isotope.

The line data of other references are less detailed than those of Kurucz. For example, Andersen et al. (1984) lists only four components of $^7\text{Li}$ and two components of $^6\text{Li}$. Smith et al. (1998) and Hobbs et al. (1999) as well as Meléndez et al. (2012) give wavelengths and $\log g f$ values for six components of $^7\text{Li}$ and three components of $^6\text{Li}$. For the purpose of comparison with the literature values quoted above, we reduced our line list for $^6\text{Li}$ from 9 to 3 components. We found only very minor wavelength differences of less than 1 mÅ, and an almost perfect agreement of the $\log g f$ values for all three $^6\text{Li}$ components. For $^7\text{Li}$, there are major differences in the $\log g f$ values of the four closely spaced red HFS components. However, they are hardly relevant since the sum of their $g f$ values is very nearly the same. We also compared our lithium line list with the data given by Morton (2003), his Table 4, and found very close agreement with the Kurucz (2006) line list regrouped to six and four components for $^7\text{Li}$ and $^6\text{Li}$, respectively.

We have double checked that the broadening parameters we used for the Li I doublet are fully consistent with the ABO theory (e.g., Barklem et al. 1998) for the van der Waals broadening and with the radiative broadening given by Kurucz (2006). Stark broadening is negligible in the temperature range considered in our investigation. We present an extended version of

### Table 2 1D-LTE Li results for $\xi$ Boo A and $\xi$ Boo B.

| BJD mid (+2450000) | $\phi$ | S/N | [M/H] solar | $^6\text{Li}/^7\text{Li}$ (%) | A(Li) (H=12) fit | $\chi^2$ fit |
|-------------------|-------|-----|-------------|-------------------------------|-----------------|---------|
| $\xi$ Boo A:      |       |     |             |                               |                 |         |
| 8609.7427427      | 0.829 | 2861 | $-0.126\pm0.0015$ | 1.448$\pm0.001$ | 2.400$\pm0.001$ | 1143    |
| 8610.8282148      | 0.998 | 2736 | $-0.127\pm0.0016$ | 1.692$\pm0.001$ | 2.400$\pm0.001$ | 1148    |
| 8611.7681903      | 0.144 | 2228 | $-0.130\pm0.0020$ | 1.872$\pm0.001$ | 2.398$\pm0.001$ | 791     |
| 8616.8333173      | 0.932 | 1688 | $-0.130\pm0.0027$ | 1.381$\pm0.001$ | 2.402$\pm0.001$ | 535     |
| 8617.6923984      | 0.066 | 2731 | $-0.130\pm0.0016$ | 1.828$\pm0.001$ | 2.400$\pm0.001$ | 1166    |
| 8617.8769492      | 0.094 | 3233 | $-0.135\pm0.0014$ | 1.779$\pm0.001$ | 2.399$\pm0.001$ | 1833    |
| 8619.7004465      | 0.378 | 2666 | $-0.126\pm0.0017$ | 1.145$\pm0.001$ | 2.399$\pm0.001$ | 1327    |
| 8619.8758547      | 0.405 | 3195 | $-0.131\pm0.0014$ | 1.283$\pm0.001$ | 2.399$\pm0.001$ | 1744    |
| **Average**       |       |     |             | $-0.129\pm0.0017$ | **1.554±0.001** | **2.400±0.001** |

| $\xi$ Boo B:      |       |     |             |                               |                 |         |
| 8609.7860453      | 0.124 | 1713 | +0.127$\pm0.002$ | ...                           | 0.367$\pm0.001$ | 5524    |
| 8610.8816143      | 0.215 | 215  | +0.138$\pm0.014$ | ...                           | 0.470$\pm0.01$  | 85      |
| 8611.8163769      | 0.294 | 1560 | +0.131$\pm0.002$ | ...                           | 0.366$\pm0.001$ | 4465    |
| 8616.8730350      | 0.717 | 1569 | +0.129$\pm0.002$ | ...                           | 0.369$\pm0.001$ | 4514    |
| 8617.8435912      | 0.798 | 1366 | +0.127$\pm0.002$ | ...                           | 0.368$\pm0.001$ | 3564    |
| 8619.7390032      | 0.957 | 1015 | +0.127$\pm0.003$ | ...                           | 0.362$\pm0.002$ | 1924    |
| **Average**       |       |     |             | +0.128$\pm0.002$ | ... | **0.366±0.003** |

BJD is barycentric-coordinate Julian date for the time of mid exposure. $\phi$ is the rotational phase based on the respective ephemeris for $\xi$ Boo A: 2,452,817.41 + 6.43 $\times$ E, and for $\xi$ Boo B: 2,452,817.41 + 11.94 $\times$ E. S/N is given for the pixel at the continuum near 6708.5 Å. Errors are always internal errors and were less than $10^{-3}$ for A(Li) for $\xi$ Boo A but were round up to $10^{-3}$ in the table. The $\chi^2$ value of the fit refers to a 130-pixels and 72-pixels range in wavelength space centered at Li I for $\xi$ Boo A and $\xi$ Boo B, respectively. $^a$without the value at fractional BJD 8610.88.
the Mott et al. (2017) Li table in the Appendix as Table A1
that also includes the broadening constants.

The ξ Boo B spectrum shows molecular contributions from various species. While CN lines are numerous included in the Meléndez et al. (2012) line list, also three C₂ blends, other molecular species are not. We are aware that several alternative line lists exist for molecular species, for example, by Brooke et al. (2014) for CN. Exploring these would be a major undertaking beyond the scope of the present study. We therefore stick to the basic list of CN and C₂ lines provided by Meléndez et al. (2012), assuming that this list would properly represent the most important features due to CN and C₂.

Table A2 presents the detailed list of atomic plus CN and C₂ lines used for the present study, including information about the broadening constants and relevant references.

A comparison with the sunspot umbral spectrum atlas of Wallace et al. (1999) for the Li range 6707.0–6708.5 Å indicates six TiO γ-band 1-0 absorptions and one line from the CaH A-band. For the TiO γ-bands (A³Φ − X³Δ) wavelengths and intensities, we refer to Ram et al. (1999). With P, Q, and R being the branches of vibrational sub-bands, all line blends for the Li region are identified belonging to these branches. The individual transitions identified by Wallace et al. (1999) are

- 6707.2 TiO γ 1-0 R₂58; 6707.3 CaH A 0-0 R₂48.5;
- 6707.4 TiO γ 1-0 R₁75; 6707.4 TiO γ 1-0 P₂27;
- 6707.8 TiO γ 1-0 Q₂40; 6708.4 TiO γ 1-0 R₂59; and
- 6708.4 TiO γ 1-0 Q₃58.

Inspired by the TiO identifications, we extracted all molecular (and atomic) lines from the VALD3 line list (Ryabchikova et al. 2015) using the default configuration, which amounts to literally thousands of TiO lines, and tried to first fit the Li-spectrum of 61 Cyg A. The plain VALD3 line list has log gf values of some prominent TiO lines that are partly too large, partly too small plus two prominent iron lines with grossly wrong log gf values which, together, resulted in unreasonable fits of the Li region of ξ Boo A. Alternatively, B. Plez privately communicated his TiO line list which is the updated version from January 2012 of the list based on Plez (1998). In McKemmish et al. (2019) this Plez-2012 line list is compared to the newer TOTO line list. At least in the wavelength range of our interest here, there seems to be a good general agreement. We combine this line list with the Meléndez et al. (2012) and Lawler et al. (2014) lists (Table A2) and employ it for the fit instead of the VALD3 list. It covers five titanium isotopes; ⁴⁶TiO with 4542 lines, ⁴⁷TiO with 4721 lines, ⁴⁸TiO with 4803 lines, ⁴⁹TiO with 4780 lines, and ⁵⁰TiO with 4695 lines. Adding all these TiO lines still allowed only for a moderate fit for 61 Cyg B and did not reveal a significant influence on the lithium fits for the initial effective temperature of ξ Boo B of 4770 K from Luck (2017). No impact whatsoever is recognizable for the fits for the even warmer ξ Boo A.

A few synthetic test runs with various effective temperatures quickly demonstrated the very steep dependency of the TiO line strength on T_eff. If ξ Boo B were cooler by 250 K, the overall TiO line strength would already increase by a factor three. At T_eff=4000 K and log g=5.0, both appropriate for a sunspot umbra according to Wallace et al. (1999), the maximum TiO line strength reached 30% of the continuum and matches the solar umbral TiO lines around Li 6707 Å very well. Only the one TiO line at 6707.45 Å appears then too deep in the synthetic spectrum by 4%. However, it does not blend with the Li lines but is included in the fitting range and thus contributes to the χ².

### 4.3 TiO band head effective temperature of ξ Boo B and 61 Cyg A

At this point we suspected that ξ Boo B’s effective temperature from Luck (2017) is too high. A comparison with a TiO spectrum of 61 Cyg A (K5V) confirms this. The TiO band head absorption at 7055 Å is markedly weaker in ξ Boo B than in 61 Cyg A. The latter is one of the Gaia benchmark stars for which a fundamental effective temperature of 4374±22 K and logarithmic gravity of 4.63±0.04 was derived from direct measurements of both angular diameter and bolometric flux (Heiter et al. 2015). Note though that the spectroscopic atomic-line determinations of T_eff arrived all at warmer temperatures; 4800 K (Heiter & Luck 2003), 4640 K (Luck & Heiter 2005), 4525 K (Affer et al. 2005), and 4545 K (Boro-Saikia et al. 2016) while an earlier determination from TiO bands suggested 4325 K (O’Neal et al. 1998). Whether cool spots can explain such temperature differences is addressed in the Appendix.

The synthetic spectra predict a line depth d of the TiO band head of d ≈ 0.45 at T_eff=4000 K (at solar metallicity for an average log g between 4.5 and 5.0). The observed line depth of the TiO band head is d ≈ 0.11 for ξ Boo B and d ≈ 0.30 for 61 Cyg A. By virtue of Eq. (3) in the Appendix, this translates to δT = (T − 4000)/1000 ≈ 0.297 and ≈ 0.101, respectively. Summarizing, we arrive at

\[
T_{\text{eff}} \approx 4300 \text{ K for } \xi \text{ Boo B},
\]

\[
T_{\text{eff}} \approx 4100 \text{ K for } 61 \text{ Cyg A}.
\]

This is to be compared to the nominal effective temperature of these stars from the literature:

\[
T_{\text{eff}} \approx 4767 \text{ K for } \xi \text{ Boo B},
\]

\[
T_{\text{eff}} \approx 4374 \text{ K for } 61 \text{ Cyg A}.
\]

In both cases, the T_eff values based on the TiO band head are significantly cooler than any of the literature temperatures. O’Neal et al. (1998) had already shown the T_eff dependency of the band head strengths based on inactive dwarf and giants
star comparison spectra. They found that TiO is most sensitive in the 3500–4000 K range. As a compromise, we will use $T_{\text{eff}} = 4570$ K for ξ Boo B.

4.4 Fitting procedure

The lithium abundance $A(\text{Li})$ and the $^6\text{Li} / ^7\text{Li}$ isotopic ratio are obtained by fitting the respective PEPSI spectrum with synthetic spectra obtained by interpolation from the pre-computed grid of synthetic line profiles. We employ the least-squares fitting algorithm MPFIT (Markwardt 2009; described in more detail in Steffen et al. 2015) included in an IDL program called TurboMPfit. TurboMPfit was designed specifically for the present purpose, that is providing the multi-dimensional library of synthetic spectra computed with Turbospectrum as input for MPFIT together with a list of fitting parameters that are to be optimized to find the minimum $\chi^2$.

The free parameters are $A(\text{Li})$, $^6\text{Li} / ^7\text{Li}$, [M/H], a global wavelength adjustment, and a global Gaussian line broadening (FWHM), which are applied in velocity space to the synthetic interpolated line profiles to match the observational data as closely as possible. FWHM represents the full width half maximum of the applied Gaussian kernel and represents the combined instrumental plus macroturbulence broadening. The continuum normalization of each spectrum is iteratively optimized initially but kept fixed at the best value in the final fits. The scaled continuum shifts with respect to the original data were $-0.002$ for ξ Boo A and $-0.020$ for ξ Boo B (and $-0.035$ for 61 Cyg A). This is in particular needed for the cool targets because the many molecular lines create a suppressed quasi continuum that the data reduction software can not handle properly. We also fit the Li doublet for all our targets using two wavelength windows; a larger range of 6706.8–6708.6 Å for normalized fluxes are simply scaled by 1+shift.

FIGURE 2 PEPSI spectrum of ξ Boo A on JD 2,458,609 (dots; left axes). Panel a. Best 1D-LTE fit (red line) for the full Li wavelength range. The fit residuals (line below) are expanded by a factor of 12.5 for better visibility (right axis). Panel b. Close up to the Li wavelength range with the best fit (dashed red line) and a comparison of two isotope ratios of 0% (black) and 10% (blue).

FIGURE 3 PEPSI spectrum of ξ Boo B on JD 2,458,609 (dots). Note the reduced fitting range 6707.3–6708.3 Å (full red line). Otherwise as in Fig. 2.
4.5 Results

The most consistent spectrum fits for ξ Boo A were achieved with stellar parameters of $T_{\text{eff}}=5480$ K, log $g=4.53$, [M/H]=−0.13, $v_{\text{micro}}=1.40$, and $v \sin i=3.0$ km s$^{-1}$. The best fits for ξ Boo B were achieved with stellar parameters of $T_{\text{eff}}=4570$ K, log $g=5.00$, [M/H]=+0.13, $v_{\text{micro}}=0.15$, and $v \sin i=1.50$ km s$^{-1}$. In the appendix, we apply also a spot model with $T_{\text{spot}}=3800$ K and a spot-area filling factor of $a = 0.3$. Note that $T_{\text{eff}}$, log $g$, and $v_{\text{micro}}$ were never solved for in our analysis but assumed fixed in the input. Combined with the observed rotation periods for both stars, above $v \sin i$ values imply minimum stellar radii of 0.38 $R_\odot$ and 0.35 $R_\odot$ for ξ Boo A and ξ Boo B, respectively. These numbers are much smaller than the nominal radii expected from the respective spectral classifications of G8V and K5V, and already hint towards a high inclination of the rotational axes with respect to the sky. The inclination of the rotation axis of ξ Boo A was indeed determined from Zeeman-Doppler imaging to $i = 28 \pm 5^\circ$ (Petit et al. 2005, Morgenthaler et al. 2012). This converts the minimum radius for ξ Boo A to a radius of 0.82 $R_\odot$, in very good agreement with its G8V classification. No observed inclination is available for ξ Boo B but, if we assume a radius of 0.66 $R_\odot$ for a K5V star as determined for 61 Cyg A (K5V) by interferometry (Kervella et al. 2008), the expected inclination for ξ Boo B would be around $\approx 32^\circ$, very similar to the observed inclination of ξ Boo A. It is now tempting to assume that the rotational axes of both components had been co-aligned over their evolutionary history. Note that there remains an inclination of $\approx 20^\circ$ with respect to AB’s joint orbital plane suggested by the orbital elements from Wielen (1962). With the mass-radius relation of Demory et al. (2009), above radii yield the most-likely masses of 0.85 $M_\odot$ and 0.68 $M_\odot$ for ξ Boo A and ξ Boo B respectively. For such low masses the standard model (Iben 1967) predicts that $^6$Li is completely destroyed early in the pre-main-sequence phase, within the first two million years.

Figures 2 and 3 show the final Li I 6708-Å line fits for one example spectrum for both ξ Boo stars without spot models. The results from all individual spectra are summarized in Table 2 with the respective numerical values for the 1D-LTE case. Grand average lithium abundances of $\Delta(\text{Li})=2.400 \pm 0.031$ and 0.37±0.09 for ξ Boo A and ξ Boo B, respectively, were derived. A 3D-NLTE correction is only available for the temperatures of ξ Boo A and is +0.05 dex (Mott et al. 2020). No such correction is available for the effective temperature of ξ Boo B. However, a simple extrapolation of the results in Mott et al. (2020) suggests a correction in the range of approximately +0.20, which would be compatible with Lind et al. (2009). Note that the error bars in Table 2 are the formal 1σ fitting errors on the free parameters, and do not indicate the final uncertainty of the measurement. The external errors given above for both $\Delta(\text{Li})$ values were estimated from the contributions of assumed uncertainties of the stellar parameters, most notably of the effective temperature of at least ±30 K, and from our previous comparison of different line lists (Mott et al. 2017). In this way, the best estimate for the external error of $\Delta(\text{Li})$ for ξ Boo A and ξ Boo B is 0.03 dex and 0.09 dex (±7% and ±23% of their respective absolute abundances), respectively, roughly 30 times the internal
fitting error. The above values of $A(\text{Li})$ make the Li abundance for the cool B-component three times less than the Sun’s, while for the A-component it is 23 times higher than the abundance of the Sun (for comparison $A(\text{Li})_{\text{Sun}} = 1.09 \pm 0.04$ dex from 3D NLTE based on PEPSI spectra of the Sun-as-a-star; Strassmeier et al. 2018a).

Global metallicities $[\text{M/H}]$ appear also significantly different for the two binary components. Our fits of the iron blend $\lambda 6707.426 \text{Å}$ suggest an average $[\text{M/H}] = -0.13 \pm 0.01$ for $\xi$ Boo A while $+0.13 \pm 0.02$ for $\xi$ Boo B. Like in the case of the Li abundance the internal errors are so small, mostly not larger than $\pm 0.002$ for $[\text{M/H}]$, that the actual external error is again dominated by the errors from $T_{\text{eff}}$, $\log g$, and the line list. The super-solar metallicity of $\xi$ Boo B is disturbing but consistently reconstructed from the Li fits. However, as long as we face massive line list uncertainties, we consider the super-solar metallicity of $\xi$ Boo B as inconclusive.

Figures 2 and 3 each show synthetic spectra with a fixed isotope ratio of 0% and 10% for comparison, along with the best-fit value as indicated in the plot. The deviations of the 10% line from the data are obvious, while no difference can be seen by eye between the best fit and the 0% assumption in case of $\xi$ Boo A. Note that the specific fit parameter $^6\text{Li}/^7\text{Li}$ was limited to values no larger than 16% for computational reasons, which was reached by the “best fit” in case of $\xi$ Boo B. However, this ratio is artificial because of the overall misfit due to yet unaccounted line contributions. Therefore, no statement regarding $\xi$ Boo B’s $^6\text{Li}$ can be made.

Finally, Fig. 4 is a comparison with the Li region of the K5V benchmark star 61 Cyg A. The spectrum was taken from Strassmeier et al. (2018b) and has $R \approx 250\,000$ and S/N of 425 per pixel. Our high-resolution spectrum of $\xi$ Boo B very much resembles that of the benchmark star 61 Cyg A, in agreement with its original K5V classification by Abt (1981) and its level of magnetic activity (Boro-Saikia et al. 2016). The same line list as for $\xi$ Boo B was employed. Adopted astrophysical parameters $T_{\text{eff}}$, $\log g$, $[\text{Fe/H}]$, $v_{\text{micro}}$, and $v \sin i$ were 4374, 4.63, +0.15, 0.84, and 0.00 in the usual units, respectively. These parameters yielded a best fit for 61 Cyg A with $A(\text{Li}) = 0.146 \pm 0.004$ (internal 1-$\sigma$ error). We also adopted a spot model for its Li fit with $T_{\text{spot}} = 3500 \text{K}$ and $a = 0.5$. The best-fit Li abundance is then $A(\text{Li}) = 0.53 \pm 0.05$ in 1D-LTE at a $\chi^2$ of 4180 for a 102-pixel range. Neither of the two approaches could fit the two $^7\text{Li}$ lines to their full line depths, opposite to the $\text{V} \text{I}$ $6708.074 \text{Å}$ and $^6\text{Li}$ $6708.077 \text{Å}$ blend. The reasons for this are likely inaccurate line parameters in the molecular and atomic line lists combined with an inhomogeneous surface temperature distribution, like for $\xi$ Boo B. We note that in the same fit the line depth of the blend $\text{Fe I}$ $6707.43 \text{Å}$ plus TiO $6707.45 \text{Å}$ was reproduced correctly (but probably at the expense of an overestimated iron abundance and macroturbulence). Significant errors in the broadening constants of the Li lines can be ruled out as an explanation for the fact that the synthetic Li lines appear to be too broad compared to the observations in the fits for $\xi$ Boo B and 61 Cyg A. Rather, this is a result of the $\chi^2$ minimization procedure defining the best fit. Presumably, the line list is incomplete or incorrect on the blue side of the Li doublet, such that the best fit is achieved with an enhanced global line broadening and a somewhat increased metallicity. Nevertheless, the two fits suggest that 61 Cyg A has a small amount of lithium left on its surface, comparable to $\xi$ Boo B.

4.6 Impact of spots

Vogt (1981) had demonstrated that the appearance of a large spot on the disk of the active star II Peg (K2 IV) caused a steep flux rise to the red and the appearance of molecular absorption features of VO and the $\gamma$ system of TiO. The most pronounced feature was the TiO $\gamma$ bandhead at 7055 Å. The differential
band head was later used as a star spot temperature diagnostic (O’Neal et al. 1998, 2004) and applied to numerous stellar targets.

Compared to the quiet Sun, the lithium equivalent width was shown to be dramatically weakened in bright plage regions and strengthened in dark sunspot umbrae (Giamapa 1984). While equivalent widths and line-strength changes are related to the low ionization potential of lithium and certainly have an additional non-radiative heating contribution from magnetic features, the Li abundance itself in these features was thus never conclusively determined or found to be non-uniform. Hultqvist (1974) theoretically explored spatial inhomogeneities of the solar lithium abundance that could result from spallation reactions during solar flares. Evidence for it was extensively searched for in more active stars than the Sun but never conclusively found (e.g., Randich et al. 1994). The spot activity in concert with the large S/N of our ξ Boo A spectra at least enable a closer look towards this issue.

We claim that if systematic deviations of the individual abundances in our time series of eight spectra follow the expected rotational modulation, then these deviations could be due to spot enhancement. No systematic deviations above 1σ were found though (Table 2), neither for component A nor component B, which places an estimated upper limit for the apparent abundance enhancement to < 0.004 dex.

5 | SUMMARY AND CONCLUSIONS

In this paper we present new spectra for both components of the visual binary ξ Boo and perform a detailed analysis of their lithium abundances with the Li i 6708-Å feature. Our new spectra are of currently highest possible quality with a two-pixel spectral resolution of 130,000 and S/N per pixel of up to 3200 for ξ Boo A and 1700 for ξ Boo B. Based on the line list of Meléndez et al. (2012), we added molecular TiO lines for the fit to the cooler B component. The same line list is also applied to a spectrum of the K5V benchmark star 61 Cyg A. While the fit to the observation is done with 1D-LTE synthetic spectra, we add a 3-D NLTE correction for ξ Boo A (none is available for the cool B component but is estimated to be of the order of +0.20 dex). Our final result is that the Li abundance of the cool B-component is at least three times less than the Sun’s, while for the A-component it is 23 times higher than the abundance of the Sun. 1D-LTE ⁷Li abundances were measured to A(Li) = 2.40 ± 0.03 dex for component A and A(Li) = 0.37 ± 0.09 dex for component B. No ⁶Li is detected for the A component, no statement is possible for the B component. At the same time the respective global metallicities also appear to be very different; the A-component has subsolar metallicity consistent with previous analyses, the B-component supersolar metallicity. While the Li difference is explainable by the different masses, effective temperatures and therefore mixing processes and efficiencies, the global metallicities should have been the same for two coeval binary components of sub-solar mass. Presumably, the metallicity of the B component is overestimated as a consequence of the incomplete line list employed for the spectrum synthesis. We consider it inconclusive at the moment. The gyrochronological age for both components is in agreement with each other and is ≈200 Myr. For 61 Cyg A we obtained a small but non-zero amount of Li of A(Li)≥0.10 dex, which increases to 0.53 dex if cool spots as large as a half a hemisphere are included. However, we emphasize that the lack of an adequate line list for stellar effective temperatures below ≈5000 K makes quantitative conclusions about the Li abundance of ξ Boo B and 61 Cyg A rather uncertain.

ξ Boo A and ξ Boo B’s lithium abundances appear in agreement with the T_{eff} and age trend found for stars in the three open clusters Pleiades, M35, and Hyades (Anthony-Twarog et al. 2018). Both our measurements very well fit the trend for M35, a cluster of subsolar metallicity and an age of ≈200 Myr, both quantities comparable to ξ Boo. In Fig. 5 we show the location of ξ Boo A and B in the A(Li) versus (B − V)_0 diagram in comparison with the lithium abundances of the various open cluster stars taken from the relevant literature. This plot clearly demonstrates that the lithium abundance of the ξ Boo binary components is fully consistent with the trend of M35, and that the gyrochronology age of the binary obtained by Barnes (2007) agrees closely with the age of this cluster. The large Li abundance difference between the two stellar components would thus be expected. Hence, neither A(Li) nor the rotation rates of the ξ Boo system appear to show any evidence for binary interaction. The non-detection of ⁷Li for ξ Boo A for a star at age ≈200 Myr simply hints toward a time scale for its depletion process that is shorter than that.

Our TiO band head simulations proved that the presence of star spots may have a significant impact on the TiO spectrum of cool stars like ξ Boo B and 61 Cyg A for both of which a substantial fraction of the stellar surface is covered by star spots. Such cool spots would certainly also affect the strength of the lithium line in a way that the Li abundance derived with a uniform model atmosphere of nominal effective temperature would likely be in error. It is therefore more appropriate to fit the Li region of stars like ξ Boo B or 61 Cyg A with a simple two-temperature spot model. Because it would not only be cool spots that contribute to a line profile (but also bright faculae or dark granulation lanes, or disk-projected prominences, a.o.), such a two-component fit may not necessarily result in a better overall fit of the observed spectrum and thus in an improved estimate of the Li abundance. Nevertheless, our Li fits for the two cool dwarfs include a pre-set spot model with reasonable
spot temperatures and spot coverage. The abundance difference $\Delta A$(Li) from a fit with and without a spot model is only small though. For $\xi$ Boo B the difference is 0.1 dex (higher abundance in case with a spot contribution) but, most important, it does not improve the fit quality. The same is true for 61 Cyg A where $\Delta A$(Li) amounts to $+0.4$ dex. At this point, we conclude that it is the line list that must be improved with many more molecules than TiO, for example, CaH, FeH, CN, a.o.. For a cool star heavily covered by magnetic-activity tracers, 3D non-LTE abundance corrections are probably a second order effect.

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APPENDIX A: LINE LISTS

APPENDIX B: OBSERVING LOG

Table B3 is the observing log for the $\xi$ Boo spectra in this paper.

APPENDIX C: CAN STAR SPOTS EXPLAIN ENHANCED TiO ABSORPTION?

In the observed spectra of $\xi$ Boo B and 61 Cyg A, the TiO lines including the TiO band head appear significantly stronger than expected from synthetic spectra computed for the nominal stellar effective temperature. Here we use synthetic spectra of the TiO 1-0 and 0-0 bands in the $\gamma$ system with band heads near 6650 Å and 7055 Å, respectively, to investigate whether star spots can be responsible for this mismatch.

C.1 Spot temperature and filling factor

A simple model assumes that we know the true effective temperature of the star, including its spots. This is in fact the case for 61 Cyg A where $T_{\text{eff}}$ is known from fundamental relations ($T_{\text{eff}} = 4374 \pm 22$ K). We then have the following relation between the fundamental $T_{\text{eff}} = T_0$, the spot temperature $T_1$, the photospheric temperature $T_2$, and the area spot filling factor $a$ in relative units of the visible stellar hemisphere

$$a T_1^4 + (1 - a) T_2^4 = T_0^4.$$  (C1)

For example, assuming $T_0 = 4374$ K like for 61 Cyg A, a spot temperature $T_1 = 4000$ K, and $a = 0.3$, we find $T_2 = 4508$ K. This value is indeed closer to the best spectroscopically determined temperatures for 61 Cyg A. Note that the Zeeman-Doppler images of 61 Cyg A in Boro-Saikia et al. (2016) can give no information on the temperature filling factor because the spectral lines are just barely broadened by rotation ($v \sin i \approx 1$ km s\(^{-1}\)) and thus do not provide spatial resolution via the Doppler effect. However, it showed magnetic fields covering large fractions of the stellar disk suggesting also a large (areal) spot filling factor.

C.2 Continuum flux and strength of TiO features

From synthetic TiO spectra computed with Turbospectrum (Plez 2012), we can derive (i) a relation between the monochromatic continuum flux and effective temperature and, (ii), a scaling relation between the normalized TiO line depth and $T_{\text{eff}}$. The following numerical relations are valid for $\log g = 4.75$. For the continuum flux, we find

$$\frac{F_\lambda(T) - F_\lambda(4 \text{ K})}{F_\lambda(4 \text{ K})} \approx 1.231 \delta T + 0.694 (\delta T)^2$$

for $\lambda = 6707$ Å, and

$$\approx 1.153 \delta T + 0.615 (\delta T)^2$$  (C2)

for $\lambda = 7055$ Å where $\delta T = (T - 4000)/1000$. For the normalized depth $d$ of (any) TiO spectral feature, we find

$$\log_{10} \left( \frac{d(T)}{d(4 \text{ K})} \right) \approx -1.75 \delta T - 1.38 (\delta T)^2 + 0.200 (\delta T)^3 + 0.369 (\delta T)^4$$
averaged over the wavelength range $\lambda = 6708.4 \pm 0.1$ Å, and

$$-1.57 \delta T - 1.55 (\delta T)^2 - 0.492 (\delta T)^3 + 0.658 (\delta T)^4$$  (C3)
TABLE A1  Twelve-component representation of the $^7$Li and $^6$Li isotopic hyper-fine structure of the lithium resonance doublet used in this work. The 19 HFS components given by Kurucz (2006) were reduced to 12 components by combining, for each isotope and fine structure component separately, hyperfine transitions of identical wavelength.

| Wavelength $\lambda$ (Å) | Lithium isotope | Excitation potential (eV) | log $gf$ (dex) | $\sigma_{ABO}$ (a.u.) | $\alpha_{ABO}$ | log $(\gamma_3/N_3)$ (cm$^3$s$^{-1}$) | log $\gamma_{rad}$ (rad s$^{-1}$) |
|------------------------|-----------------|---------------------------|--------------|---------------------|------------|-------------------------------|-------------------------------|
| 6707.756               | $^7$Li          | 0.000                     | -0.428       | 346                 | 0.236     | -5.78                          | 7.567                         |
| 6707.768               | $^7$Li          | 0.000                     | -0.206       | 346                 | 0.236     | -5.78                          | 7.567                         |
| 6707.907               | $^7$Li          | 0.000                     | -0.808       | 346                 | 0.236     | -5.78                          | 7.567                         |
| 6707.908               | $^7$Li          | 0.000                     | -1.507       | 346                 | 0.236     | -5.78                          | 7.567                         |
| 6707.919               | $^7$Li          | 0.000                     | -0.808       | 346                 | 0.236     | -5.78                          | 7.567                         |
| 6707.920               | $^7$Li          | 0.000                     | -0.808       | 346                 | 0.236     | -5.78                          | 7.567                         |
| 6707.920               | $^6$Li          | 0.000                     | -0.479       | 346                 | 0.236     | -5.78                          | 7.567                         |
| 6707.923               | $^6$Li          | 0.000                     | -0.178       | 346                 | 0.236     | -5.78                          | 7.567                         |
| 6708.069               | $^6$Li          | 0.000                     | -0.831       | 346                 | 0.236     | -5.78                          | 7.567                         |
| 6708.070               | $^6$Li          | 0.000                     | -1.734       | 346                 | 0.236     | -5.78                          | 7.567                         |
| 6708.074               | $^6$Li          | 0.000                     | -0.734       | 346                 | 0.236     | -5.78                          | 7.567                         |
| 6708.075               | $^6$Li          | 0.000                     | -0.831       | 346                 | 0.236     | -5.78                          | 7.567                         |

Notes: $^a$ at $T = 10000 K$; van der Waals broadening parameters $\sigma_{ABO}$ and $\alpha_{ABO}$ from Barklem et al. (2000); all other data from references specified in Kurucz (2006).

averaged over the wavelength range $\lambda = 7055 \pm 1$ Å. The latter equation can be used to derive a formal effective temperature from the strength of the TiO band head. Figure C1 is a direct comparison of the band head strengths for ξ Boo B and 61 Cyg A with synthetic spectra for various effective temperatures.

### C.3 Starspot contribution

We investigate a simple model assuming that a fraction $a$ of the stellar surface is covered by spots with a lower temperature $T_1$, while the rest of the stellar surface radiates with effective temperature $T_2$. Using the above relations, we can then estimate the strength of the TiO absorption in the combined spectrum, $\overline{d}$. The following relation holds for the line depth of the combined spectrum

$$
\overline{d} = \frac{a F_{\lambda,1} d_1 + (1-a) F_{\lambda,2} d_2}{a F_{\lambda,1} + (1-a) F_{\lambda,2}} = \frac{a R_1 d_1 + (1-a) d_2}{a R_1 + (1-a)} \quad \text{Eq. (C4)}
$$

where $F_{\lambda,1}$ and $F_{\lambda,2}$ denote the monochromatic continuum flux in the spots and the quiet photosphere, respectively. $R_1 = F_{\lambda,1}/F_{\lambda,2}$, and $d_1$ and $d_2$ refer to the normalized line depth in the local spectra of the two components. Note that completely dark spots ($R_1 = 0$) would not have any impact on the combined spectrum, $\overline{d} = d_2$. Obviously, there is a certain optimum spot temperature where the spectral signature of the star spots is at its maximum.

### C.3.1 Results for 61 Cyg A

Given the mean (true) effective temperature of the star, $T_{\text{eff}} = T_0$, we can now compute $\overline{d}$ for any combination of $a$ and $T_1$. First we obtain $T_2$ from Eq. (C1). Then the continuum fluxes $F_{\lambda,1}$ and $F_{\lambda,2}$ are obtained from Eq. (C2) and the local line depths from Eq. (C3). Finally, these quantities are used to evaluate $\overline{d}$ from Eq. (C4).

Adopting $T_{\text{eff}} = 4374 K$, the observed strength of the TiO band head ($\overline{d} \approx 0.3$) can only be explained by the presence of star spots if they are cooler than about 3500 K and cover at least half of the visible stellar surface. The latter is not obvious for a star with only a low modulation amplitude in Ca II H&K and a rotation period of 35.7 d (Boro-Saikia et al. 2016) unless the cool spots are evenly distributed across stellar longitudes and remain like that.

Figure C2 shows the spot-model Li fit for 61 Cyg A. Shown is the fit with $T_{\text{eff}} = T_0 = 4374 K$, a spot temperature of 3500 K, and a filling factor $a$ of 0.5. The Li abundance from this fit is A(Li) = 0.53 dex. Figure C2 can be directly compared with the non-spot results in Fig. 4p. A considerable shift in flux scale can be noted ($-0.07$). Table C4 is an excerpt of spot models with two rather extreme spot filling factors of $a = 0.5$ and $a = 0.6$. We also note that the fits including spots require super-solar metallicity but with a slightly lowered level of [Fe/H]≈0.037 dex than for the non-spot fit.
TABLE A2  List of atomic and molecular lines in the Li 6707Å region. Wavelength, excitation potential, and log gf values adopted from [2012], except for the V 1 line. For atomic lines (except V 1), the van der Waals broadening parameter $\gamma_6$ is computed by the Unsöld approximation with line-specific enhancement factors; Stark broadening is ignored.

| Wavelength (Å) | Chemical species | Excitation pot. (eV) | log gf (dex) | References for $\lambda$ and log gf | log($\gamma_6/N_H$) | $f_{\text{damp}}$ | log $\gamma_{\text{rad}}$ |
|---------------|-----------------|----------------------|-------------|----------------------------------|-----------------|------------|-------------------|
| 6707.000      | Si I            | 5.954                | -2.560      | Mandell et al. (2004)            | -6.812          | 1.3        | 8.146             |
| 6707.172      | Fe I            | 5.538                | -2.810      | Mandell et al. (2004)            | -6.919          | 1.6        | 8.176             |
| 6707.433      | Fe I            | 4.608                | -2.250      | Mandell et al. (2004)            | -7.306          | 1.5        | 8.301             |
| 6707.473      | Sm II           | 0.933                | -1.910      | Xu et al. (2003)                 | -7.575          | 1.0        | 5.483             |
| 6707.596      | Cr I            | 4.208                | -2.667      | Mandell et al. (2004)            | -6.784          | 10.0       | 7.176             |
| 6708.023      | Si I            | 6.000                | -2.800      | Kurucz (2007, VALD)              | -6.762          | –          | 8.146             |
| 6708.110      | V I             | 1.218                | -2.630      | Lawler et al. (2014)             | 331.245         | –          | 7.602             |
| 6708.099      | Ce II           | 0.701                | -2.120      | Palmeri et al. (2000)            | -7.576          | 1.0        | 4.972             |
| 6708.282      | Fe I            | 4.988                | -2.700      | Mandell et al. (2004)            | -7.188          | 1.3        | 6.672             |
| 6708.347      | Fe I            | 5.486                | -2.580      | Mandell et al. (2004)            | -6.954          | 1.5        | 7.968             |
| 6708.534      | Fe I            | 5.558                | -2.936      | Mandell et al. (2004)            | -6.905          | 1.4        | 8.301             |
| 6708.577      | Fe I            | 5.446                | -2.684      | Mandell et al. (2004)            | -6.979          | 1.4        | 8.477             |
| 6707.205      | CN              | 1.970                | -1.222      | Mandell et al. (2004)            | -              | –          | 6.176             |
| 6707.272      | CN              | 2.177                | -1.416      | Meléndez & Barbuy (1999)         | –              | –          | 6.176             |
| 6707.282      | CN              | 2.055                | -1.349      | Meléndez & Barbuy (1999)         | –              | –          | 6.176             |
| 6707.300      | C$_2$           | 0.933                | -1.717      | Meléndez & Cohen (2007),         | –              | –          | 6.771             |
|               |                 |                      |             | Meléndez & Asplund (2008)        | –              | –          | 6.771             |
| 6707.371      | CN              | 3.050                | -0.522      | Mandell et al. (2004)            | –              | –          | 6.176             |
| 6707.460      | CN              | 0.788                | -3.094      | Meléndez & Barbuy (1999)         | –              | –          | 6.176             |
| 6707.461      | CN              | 0.542                | -3.730      | Meléndez & Barbuy (1999)         | –              | –          | 6.176             |
| 6707.470      | CN              | 1.880                | -1.581      | Mandell et al. (2004)            | –              | –          | 6.176             |
| 6707.548      | CN              | 0.946                | -1.588      | Meléndez & Barbuy (1999)         | –              | –          | 6.176             |
| 6707.595      | CN              | 1.890                | -1.451      | Mandell et al. (2004)            | –              | –          | 6.176             |
| 6707.645      | CN              | 0.946                | -3.330      | Meléndez & Barbuy (1999)         | –              | –          | 6.176             |
| 6707.660      | C$_2$           | 0.926                | -1.743      | Meléndez & Cohen (2007),         | –              | –          | 6.771             |
|               |                 |                      |             | Meléndez & Asplund (2008)        | –              | –          | 6.771             |
| 6707.809      | CN              | 1.221                | -1.935      | Meléndez & Barbuy (1999)         | –              | –          | 6.176             |
| 6707.848      | CN              | 3.600                | -2.417      | Mandell et al. (2004)            | –              | –          | 6.176             |
| 6707.899      | CN              | 3.360                | -3.110      | Mandell et al. (2004)            | –              | –          | 6.176             |
| 6707.930      | CN              | 1.980                | -1.651      | Mandell et al. (2004)            | –              | –          | 6.176             |
| 6707.970      | C$_2$           | 0.920                | -1.771      | Meléndez & Cohen (2007),         | –              | –          | 6.771             |
|               |                 |                      |             | Meléndez & Asplund (2008)        | –              | –          | 6.771             |
| 6707.980      | CN              | 2.372                | -3.527      | Meléndez & Barbuy (1999)         | –              | –          | 6.176             |
| 6708.026      | CN              | 1.980                | -2.031      | Mandell et al. (2004)            | –              | –          | 6.176             |
| 6708.147      | CN              | 1.870                | -1.884      | Mandell et al. (2004)            | –              | –          | 6.176             |
| 6708.315      | CN              | 2.640                | -1.719      | Mandell et al. (2004)            | –              | –          | 6.176             |
| 6708.370      | CN              | 2.640                | -2.540      | Mandell et al. (2004)            | –              | –          | 6.176             |
| 6708.420      | CN              | 0.768                | -3.358      | Meléndez & Barbuy (1999)         | –              | –          | 6.176             |
| 6708.541      | CN              | 2.500                | -1.876      | Mandell et al. (2004)            | –              | –          | 6.176             |

$^a$ at $T = 10000$ K; $^b$ van der Waals damping enhancement factor relative to VALD3 (2022) where applicable; $^c$ Radiative damping constants $\gamma_{\text{rad}}$ are from the VALD3 database (2021); $^d$ notation for $\sigma_{\text{ABO}} = 331$ and $\alpha_{\text{ABO}} = 0.245$; $^e$ no van der Waals broadening is applied for molecular lines; $^1$ $\lambda$ and/or log gf presumably adjusted by Meléndez et al. (2012) to better reproduce the solar spectrum; $^2$ see also Kotlar et al. (1989); $^3$ see also Jørgensen & Larsson (1990).
| BJD mid exp. (+2450000) | $\phi$ (Eq. 1) | $t_{\text{exp}}$ (min) | $\Delta t$ (min) | $\Delta \lambda$ (blue; red) | S/N p. pixel blue | red |
|-------------------------|----------------|------------------------|-----------------|-----------------------------|------------------|-----|
| Boo A: |
| 8609.7427427            | 0.829          | 5                      | 38              | 4800-5441; 6278-7419         | 2150             | 2980 |
| 8610.8282148            | 0.998          | 5                      | 38              | 4800-5441; 6278-7419         | 2020             | 2910 |
| 8611.7681903            | 0.144          | 5                      | 38              | 4800-5441; 6278-7419         | 1590             | 2390 |
| 8616.8333173            | 0.932          | 5                      | 38              | 4800-5441; 6278-7419         | 1170             | 1770 |
| 8617.6923984            | 0.066          | 5                      | 38              | 4800-5441; 6278-7419         | 2120             | 2850 |
| 8617.8769492            | 0.094          | 5                      | 38              | 4800-5441; 6278-7419         | 2450             | 3380 |
| 8619.7004465            | 0.378          | 5                      | 38              | 4800-5441; 6278-7419         | 1970             | 2800 |
| 8619.8758547            | 0.405          | 5                      | 38              | 4800-5441; 6278-7419         | 1370             | 3360 |
| Boo B: |
| 8609.7860453            | 0.124          | 10                     | 68              | 4800-5441; 6278-7419         | 990              | 1850 |
| 8610.8816143            | 0.215          | 10                     | 68              | 4800-5441; 6278-7419         | 300              | 240 |
| 8611.8163769            | 0.294          | 10                     | 68              | 4800-5441; 6278-7419         | 890              | 1720 |
| 8616.8730350            | 0.717          | 10                     | 68              | 4800-5441; 6278-7419         | 870              | 1710 |
| 8617.8435912            | 0.798          | 5                      | 38              | 4800-5441; 6278-7419         | 710              | 1470 |
| 8619.7390032            | 0.957          | 10                     | 68              | 4800-5441; 6278-7419         | 560              | 1080 |

The first column gives the barycentric Julian date for the time of mid exposure for Stokes I. The second column is the rotational phase $\phi$ based on the respective ephemeris for $\xi$ Boo A and for $\xi$ Boo B. Six individual exposures with an exposure time $t_{\text{exp}}$ and a total cadence of $\Delta t$ (both in minutes) make up one phase spectrum. S/N is per pixel and is an average from the respective wavelength region $\Delta \lambda$ (dubbed blue and red). $a$. Bad weather. $b$. Exposure time was accidentally set to 4 min in the blue, and to 5 min in the red.
FIGURE C1 Comparisons of observed and synthetic spectra of the TiO γ 0-0 band head at λ 7055 Å. For comparison with ξ Boo B (top panel, thick line) and 61 Cyg A (bottom panel, thick line), the synthetic spectra have been broadened with a Gaussian of FWHM=4.0 and 2.0 km/s, respectively, roughly representing the effect of instrumental broadening plus macro turbulence. The effective temperature of the superimposed synthetic spectra are chosen to bracket the observed strength of the TiO lines. In all cases, we adopt log g = 4.5 and solar metallicity.
FIGURE C2 1D-LTE fits for 61 Cyg A for three isotope ratios (lines as labeled) and a spot model with $T_{\text{spot}} = 3500$ K, and a filling factor $a$ of 0.5. Otherwise as in Fig. 4 b.

TABLE C4 TiO band head at 7055 Å for star spot model of 61 Cyg A ($T_{\text{eff}}=4374$ K)

| $a$ | $T_1$ | $T_2$ | $R_j$ | $d_1$ | $d_2$ | $\bar{d}$ |
|-----|-------|-------|-------|-------|-------|---------|
|     |       |       |       |       |       |         |
| 0.500 | 4374  | 4374  | 1.000 | 0.068 | 0.068 | 0.068   |
| 0.500 | 4300  | 4444  | 0.858 | 0.108 | 0.043 | 0.073   |
| 0.500 | 4200  | 4529  | 0.704 | 0.188 | 0.023 | 0.091   |
| 0.500 | 4100  | 4604  | 0.584 | 0.302 | 0.013 | 0.119   |
| 0.500 | 4000  | 4671  | 0.488 | 0.450 | 0.008 | 0.153   |
| 0.500 | 3900  | 4730  | 0.411 | 0.624 | 0.005 | 0.185   |
| 0.500 | 3800  | 4783  | 0.349 | 0.814 | 0.003 | 0.213   |
| 0.500 | 3700  | 4830  | 0.298 | 1.009 | 0.002 | 0.233   |
| 0.500 | 3600  | 4873  | 0.258 | 1.209 | 0.001 | 0.249   |
| 0.500 | 3500  | 4911  | 0.226 | 1.427 | 0.001 | 0.264   |

|     |       |       |       |       |       |         |
| 0.600 | 4374  | 4374  | 1.000 | 0.068 | 0.068 | 0.068   |
| 0.600 | 4300  | 4444  | 0.858 | 0.108 | 0.034 | 0.075   |
| 0.600 | 4200  | 4601  | 0.655 | 0.188 | 0.013 | 0.100   |
| 0.600 | 4100  | 4707  | 0.528 | 0.302 | 0.006 | 0.137   |
| 0.600 | 4000  | 4800  | 0.432 | 0.450 | 0.003 | 0.178   |
| 0.600 | 3900  | 4881  | 0.357 | 0.624 | 0.001 | 0.219   |
| 0.600 | 3800  | 4953  | 0.299 | 0.814 | 0.001 | 0.252   |
| 0.600 | 3700  | 5017  | 0.253 | 1.009 | 0.000 | 0.278   |
| 0.600 | 3600  | 5074  | 0.216 | 1.209 | 0.000 | 0.296   |
| 0.600 | 3500  | 5125  | 0.188 | 1.427 | 0.000 | 0.314   |
C.3.2 Results for ξ Boo B

Figure C3 shows the spot-model fit for ξ Boo B. Shown is the fit with $T_{\text{eff}} = T_0 = 4570$ K, a spot temperature of 3800 K, and a filling factor $a$ of 0.3. The Li abundance from this fit is $A(\text{Li}) = 0.45$ dex. The plot can be directly compared with the non-spot fit in Fig. 3 b. Here, the shift in flux scale is $-0.02$. Table C5 is an overview of selected results for ξ Boo B, always assuming an effective temperature of 4570 K. According to these results, the observed strength of the TiO band head ($d \approx 0.1$) can be explained by different star spot configurations. For a filling factor of 0.3, the spots must have a temperature of about 3800 K. For larger filling factors of $a = 0.4$ or even 0.5, the necessary spot temperature would be 3900 K and 4000 K, respectively.

As for 61 Cyg A, we note that the fits including a spot model still require super-solar metallicity but with a slightly lowered level of [Fe/H] ≈ 0.085 dex.

C.3.3 Results for ξ Boo A

In this case, we focus only on the strong TiO line at $\lambda 6708.4$ Å in the lithium region which, like the 7055 Å band head, is not detected in our observed spectra of ξ Boo A. This constrains the spot properties of this star. The results of our simple star spot model for $T_{\text{eff}} = T_0 = 5480$ K indicate that spots must not be cooler than about 4000 K if the filling factor is in the range 0.1 . . . 0.2. Even larger filling factors, $a > 0.25$, require $T_1 > 4200$ K. Otherwise this TiO line would be visible in the high-resolution PEPSI spectrum with a line depth of about 1%, which is not the case.

| $a$ | $T_1$ | $T_2$ | $R_\lambda$ | $d_1$ | $d_2$ | $\overline{d}$ |
|-----|-------|-------|-------------|------|------|---------------|
|     |       |       |             | 0.017 | 0.017 | 0.017         |
| 0.300 | 4570 | 4570 | 1.000 | 0.017 | 0.017 | 0.017         |
| 0.300 | 4500 | 4599 | 0.905 | 0.029 | 0.014 | 0.018         |
| 0.300 | 4400 | 4637 | 0.786 | 0.058 | 0.010 | 0.022         |
| 0.300 | 4300 | 4672 | 0.683 | 0.108 | 0.008 | 0.030         |
| 0.300 | 4200 | 4704 | 0.593 | 0.188 | 0.006 | 0.043         |
| 0.300 | 4100 | 4733 | 0.516 | 0.302 | 0.005 | 0.058         |
| 0.300 | 4000 | 4760 | 0.448 | 0.450 | 0.003 | 0.076         |
| 0.300 | 3900 | 4784 | 0.391 | 0.624 | 0.002 | 0.092         |
| 0.300 | 3800 | 4806 | 0.341 | 0.814 | 0.001 | 0.106         |
|     |       |       |             | 0.017 | 0.017 | 0.017         |
| 0.400 | 4570 | 4570 | 1.000 | 0.017 | 0.017 | 0.017         |
| 0.400 | 4500 | 4599 | 0.905 | 0.029 | 0.014 | 0.018         |
| 0.400 | 4400 | 4637 | 0.786 | 0.058 | 0.010 | 0.022         |
| 0.400 | 4300 | 4672 | 0.683 | 0.108 | 0.008 | 0.030         |
| 0.400 | 4200 | 4704 | 0.593 | 0.188 | 0.006 | 0.043         |
| 0.400 | 4100 | 4733 | 0.516 | 0.302 | 0.005 | 0.058         |
| 0.400 | 4000 | 4760 | 0.448 | 0.450 | 0.003 | 0.076         |
| 0.400 | 3900 | 4784 | 0.391 | 0.624 | 0.002 | 0.092         |
| 0.400 | 3800 | 4806 | 0.341 | 0.814 | 0.001 | 0.106         |
|     |       |       |             | 0.017 | 0.017 | 0.017         |
| 0.500 | 4570 | 4570 | 1.000 | 0.017 | 0.017 | 0.017         |
| 0.500 | 4500 | 4599 | 0.905 | 0.029 | 0.010 | 0.019         |
| 0.500 | 4400 | 4637 | 0.724 | 0.058 | 0.005 | 0.027         |
| 0.500 | 4300 | 4799 | 0.606 | 0.108 | 0.003 | 0.042         |
| 0.500 | 4200 | 4867 | 0.510 | 0.188 | 0.001 | 0.064         |
| 0.500 | 4100 | 4928 | 0.432 | 0.302 | 0.001 | 0.092         |
| 0.500 | 4000 | 4982 | 0.367 | 0.450 | 0.001 | 0.121         |
| 0.500 | 3900 | 5031 | 0.314 | 0.624 | 0.000 | 0.149         |
| 0.500 | 3800 | 5075 | 0.269 | 0.814 | 0.000 | 0.173         |