A VAPID analysis of interstellar lithium in the ζ Oph sightline

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ABSTRACT

We present observations of the Li I 6708 Å doublet in the ζ Oph sightline, obtained at a resolution of ~10⁶ and a signal-to-noise ratio of ~1200, together with supplementary observations of K I λ7699 and the Na I λ3302 doublet. These observations marginally resolve the main ‘ ~15 km s⁻¹ system into its two principal clouds; we model the data using standard physical assumptions, but in a statistically rigorous manner, taking fully into account the hyperfine, doublet and isotopic structure for each species, in each cloud, using a new code, VAPID. The average ⁷Li/⁶Li ratio determined in this sightline is 1.12 ± 0.20 dex (68 per cent confidence interval), in excellent agreement with the solar-system (meteoritic) value. The ratios in the individual clouds are determined with less precision, but are also consistent with the solar-system value, as is the total lithium abundance (with little evidence for depletion). The thermal and ‘turbulent’ broadening in the two clouds is discussed on the basis of observed line widths.

Key words: stars: individual: ζ Ophiuchi (HD 149757) – ISM: atoms.

1 INTRODUCTION

Of the light elements, lithium is of particular interest as a potential diagnostic of conditions in the Universe at the epoch of primordial nucleosynthesis, and of stellar and galactic chemical evolution (e.g. Ryan et al. 2001). The total lithium abundance, ⁶Li + ⁷Li, has been extensively studied in the atmospheres of cool stars, leading to the identification of the ‘Spite plateau’, [Li/H] = −1.1, with the primordial lithium abundance (Spite & Spite 1982a,b). However, the interpretation of stellar abundances relies on relatively complex radiative transfer, and on the degree of processing of photospheric lithium.²

The relatively fragile ⁶Li isotope is not produced in significant quantities in standard models of big-bang nucleosynthesis, and therefore offers an insight into lithium production processes such as spallation and stellar nucleosynthesis (and hence into the production of other light elements, such as Be and B; e.g., Steigman & Walker 1992; Lemoine, Vangioni-Flam & Cassé 1998; Parizot 2000), and perhaps even into the ingestion of planetary bodies by stars (Alexander 1967; Israelian et al. 2001). Observationally, the ⁶Li abundance is extremely difficult to measure in stellar atmospheres, with only five successful determinations published at the time of writing (e.g. Smith, Lambert & Nissen 1993, 1998; Cayrel et al. 1999; Nissen et al. 1999; Israelian et al. 2001). In general, therefore, the interstellar medium (ISM) offers wider opportunities for testing models of the evolution of lithium abundance through the isotopic abundance ratio. Furthermore, the neutral-atom isotopic ratio ⁷Li/⁶Li is insensitive to many potential systematic uncertainties in the determination of absolute lithium abundances, to depletion from the gas phase on to dust grains in the ISM and to uncertainties in ionization fractions, making it a particularly useful diagnostic (e.g. Steigman et al. 1993).

Unfortunately, the only resonance lines accessible from the ground, the Li I λ6708 doublet, are generally rather weak (the dominant ion in the diffuse ISM being Li⁺); moreover, the doublet separation is comparable to the isotopic separation (~0.15 and 0.16 Å, respectively), so there is inevitably overlap between ⁶Li and ⁷Li lines. Thus both high resolution and high signal-to-noise ratio are required in order to allow satisfactory modelling. These observational difficulties are reflected in previous (and our own) efforts to measure the ⁷Li/⁶Li ratio towards ζ Oph.

Although there are at least 12 distinct absorption components in this sightline (Barlow et al. 1995; Welty, Hobbs & Kulkarni 1994), more than 90 per cent of absorbers are contained in two clouds at ³
−14.0 and −15.0 km s$^{-1}$, and this ‘−15 km s$^{-1}$ blend’ is the
dominant feature in lithium. Ferlet & Dennefeld (1984) failed to
detect $^6$Li in this feature, and inferred $^7$Li/$^6$Li ≈ 38 (≈ 25). Meyer,
Hawkins & Wright (1993) subsequently found a very different
value, $^{6,7}$Li = 14, a result that Lemoine, Ferlet & Vidal-Madjar (1995)
criticized as being an average over unresolved components.
However, Lemoine et al. in turn failed to model the $−15$ km s$^{-1}$
blend as a close pair of components, even though the velocity
structure was already established at the time of their work
(Le Bourlet, Gérin & Pérault 1989; Lambert, Sheffer & Crane
1990; Crawford et al. 1994). None the less, in a very thorough
study, they concluded that any unmodelled structure was unlikely
to affect their results significantly. They derived $^7$Li/$^6$Li ratios of
8.6 ± 0.8 (± 1.4 systematics) and $1.4$ ± 0.5 (± 1.4) for the
−$15$ km s$^{-1}$ blend and −$19$ km s$^{-1}$ cloud, respectively, from
spectra with a resolution of 10$^9$ and a signal-to-noise ratio of 7500
(stochastic). The present work re-examines the ζ Oph spectrum at
higher resolution, in an effort to determine improved values for the
lithium isotope ratio in this sightline, and to investigate whether the
results are consistent with the solar-system (meteoritic) value of
$^7$Li/$^6$Li = 12.3 (Anders & Grevesse 1989).

2 OBSERVATIONS

The principal data set discussed here consists of observations
obtained during 1994 June, using the ultra-high-resolution facility
(UHRF) at the 3.9-m Anglo-Australian Telescope (AAT). The data
were extracted in the standard manner using FIGARO routines
(Shortridge et al. 1999).

The detector was a Tektronix charge-coupled device (CCD) with
1024 × 1024 × 24-μm$^2$ pixels. The data have been flat-fielded, but
it should be noted that the CCD had good cosmetic properties, and
that with UHRF the spectrum is spread over 456 detector pixels in
the spatial direction (binned on-chip × 8), which considerably
reduces the effects of pixel-to-pixel variations in sensitivity. To
mitigate the effects of possible instrumental signatures yet further,
54 separate 1200-s integrations of ζ Oph were obtained in groups
of observations with offset central wavelengths. Observations of α
Aql and α Vir were obtained to investigate the effect of weak
telluric lines; in common with previous workers, we find no
evidence that telluric absorption is a significant contaminant of the
lithium spectrum.

The total of 18-h integration on the lithium lines yielded a
continuum signal-to-noise ratio of $\sim$1200 per wavelength bin, as
determined empirically from low-order polynomial fits to the
continuum. Supplementary observations of the much stronger Kτ
$\lambda$7699 line were obtained at lower signal-to-noise ratio (S/N
ratio = 100). The resolution in the reduced spectra, determined
from measurements of a stabilized He–Ne laser line, is
0.34 km s$^{-1}$ (FWHM, $R = 8.8 \times 10^5$), with the data sampled
every 0.16 km s$^{-1}$. In addition, we have used observations of the
Na ultraviolet (UV) doublet (λ3302, 3303) reported by Barlow
et al. (1995). Those observations, which have a continuum S/N
ratio of $\sim$40, were taken during commissioning of UHRF, before
the instrument was fully optimized, and suffer, in particular, from
uncertainty in the zero-point of the intensity scale at the $\sim$10 per
cent level.

3 THE VAPID MODELLING TOOL

We have developed new software to model interstellar absorption
lines, under the customary assumptions of a Gaussian line-of-sight
velocity distribution$^4$ of pure absorbers in each ‘cloud’ (Strömgren
1948). With these assumptions a cloud is fully specified by a
central velocity, column density and velocity dispersion. We follow
standard practice by giving the column density, $N$, in cgs units, and
by using $b$ to characterize the velocity dispersion, where $b/\sqrt{2}$ is the
rms line-of-sight particle velocity (and the rms space velocity for
the Maxwellian distribution is $b/\sqrt{3/2}$). The FWHM of an
unsaturated line is $2b/\sqrt{n}$.

The Voigt functions required for the modelling are generated
with Lysnas-Gray’s voigt1 routine (Lysnas-Gray 1993), and
optimization of parameter values is performed with an extensively
customized version of Press et al.’s implementation of the Marquadt
algorithm (Press et al. 1992). The remainder of the program ($\sim$90
per cent of $\sim$6000 lines of code) provides the control logic, user
interface, checks, error and statistical analysis, etc. The code is
called VAPID, which can be taken to be an acronym for Voigt
Absorption Profile (Interstellar) Dabbler.$^5$

Operationally, a distinctive feature of VAPID is that it allows
cloud parameters to be optimized with respect to several different
data sets simultaneously; those data sets may include observations
of different transitions of a given species, and may have different
S/N ratios and resolutions. Because wavelength calibrations are not
of indefinite accuracy, a least-squares adjustment of the velocity
zero-points (with respect to a selected reference spectrum) is
normally included when optimizing a model with respect to
multiple data sets. (This is particularly important for UHRF data
sets, where the high dispersion means that only two or three useful
lines may be recorded in the calibration arc, with the wavelength
accuracy consequently being limited by the reliability of the
tabulated arc-line wavelengths.)

The least-squares optimization automatically yields estimates of
the uncertainties on derived parameters in the standard way, from
the covariance matrix, after data errors have been rescaled to
ensure a reduced $\chi^2$ of unity in regions where the synthesized
spectrum falls below a specified residual intensity ($0.9999$ by
default). As is well known, these ‘single-parameter’ error estimates
can be significantly smaller than their ‘multiparameter’ counterparts.
To obtain realistic, non-parametric error estimates, the
analyst may use VAPID to investigate the distributions of parameter
values by bootstrap or Monte Carlo methods.$^6$

In principle, the bootstrap approach is preferable; in practice,
observations often sample interstellar absorption lines rather poorly,
encouraging the use of Monte Carlo methods, whereby artificial data
sets are generated from the original data and their errors. An
advantage of the Monte Carlo approach is that it is straightforward
to incorporate additional information (for example, the estimated size
of systematic errors in the continuum and zero-intensity levels) when
generating the replicated data sets. In practice, our experience (with
many data sets in addition to that discussed here) is that the
‘multiparameter’ error estimates are often not more than a few tens
of per cent larger than their ‘single-parameter’ counterparts.

The statistical information from an optimization can be used to
address two related questions: first, is the fit ‘good’, and secondly,

$^4$ Consistent with, but not requiring, a Maxwellian three-dimensional
velocity distribution.

$^5$ To dabble is ‘to do anything in a trifling or small way’ (Macdonald 1972).

$^6$ To be explicit, for a given variable, a ‘single-parameter, 1σ error estimate
is obtained from the 68 per cent of replicated data sets that give solutions for that variable
which are closest to the original least-squares solution; a
‘multiparameter, 1σ error estimate is obtained from the 68 per cent of replications which yield the smallest values for $\chi^2$. 

is the improvement in $\chi^2$ resulting from the addition of extra components ‘significant’? In each case answers can be obtained by comparing variances, with the F-test; in the first case, $\chi^2$ can be compared within and outside the line (where ‘the line’ is chosen to be those regions where the optimized model spectrum falls below the continuum).

In the second case, if an initial model with $n_1$ free parameters yields a chi-squared of $\chi_1^2$, and a second model with $n_2 = n_1 + \Delta n$ free parameters yields $\chi_2^2$ (where $\Delta n$ will usually be 3 for each additional cloud), then

$$\frac{\chi_2^2 - \chi_1^2 N - n_1}{\Delta n}$$

is distributed as $F[\Delta n, (N - n_1)]$, where $N$ is the number of data points in the line. A large value of $F$ means that the extra terms give a ‘significantly’ improved fit, where the level of significance can be assessed from standard tables of $F$ (noting that the appropriate distribution is one-tailed; the test is to see whether there is an improvement, not merely a change, in $\chi^2$).

4 ANÁLISIS: ζ OPH

4.1 Lithium: comparison with previous analyses

We begin by comparing previous models of the lithium lines with our observations; this comparison is made in Fig. 1. Here, as elsewhere in this paper, we take into account hyperfine structure, with the simplification that each doublet component is split into two hyperfine components (thereby neglecting hyperfine splitting of the upper levels). For lithium, we use wavelengths determined by Sansonetti et al. (1995); otherwise, we adopt atomic data summarized by Welty et al. (1994). Unfortunately, Welty et al. do not give primary sources, but their oscillator strengths are identical to those listed by Morton (1991), who does give sources. The wavelengths of Sansonetti et al. for lithium differ from those given by Welty et al. by less than 0.1 km s$^{-1}$.

Meyer et al. (1993, hereinafter MHW) used a single-cloud model and simply fitted appropriately constrained Gaussians to their observations. While this is a reasonable approximation to the profiles of very optically thin lines, such as those considered here, MHW do not give their best-fitting Gaussian parameters, so that their observations are not readily summarized in terms of the usual $\{v, b, N\}$ triplet. The model shown in Fig. 1 therefore uses the isotopic ratio given by MHW, but with $v_\ast$, $b$ and $N(\text{Li}^\text{b})$ as optimized parameters. Lemoine et al. (1995, hereinafter LFV) parametrized their fit with the standard physical model used here, so only the central velocity of the system, $v_\ast$, is optimized (to accommodate small velocity zero-point shifts between their observations and ours).

For the purposes of comparison, we have modelled our UHRF observations with a single-cloud model; the best-fitting parameters for this model are included in Table 1 (Model Li$\ast$−1). The resulting $^6\text{Li}^\text{b}/\text{Li}$ ratio, 1.09$^{+0.12}_{-0.10}$ dex, is identical to the solar-system value reported by Anders & Grevesse (1989), and is slightly larger than the values given by MHW ($0.83 \pm 0.11$) and LFV ($0.93 \pm 0.04$ statistical, $\pm 0.08$ systematic). The differences are acceptable to within the quoted errors, and are evidently largely attributable to the $\lambda 6708.072$ line of $^6\text{Li}$ appearing slightly weaker in our spectrum (central depth $\sim99.9$ per cent of the continuum level). Of course, the $^7\text{Li}$ column is additionally constrained by the $\lambda 6707.912$ doublet component, although that component is irresolvably blended with the hyperfine-split $\lambda\lambda 6707.905, 6707.917$ doublet component in $^7\text{Li}$. (In the optically thin limit, $^7\text{Li}$ reveals its presence by an apparent $^7\text{Li}$ doublet ratio of less than 2. In our data, that ratio is $\sim 1.7$.)

At the level expected from LFV’s modelling, the −19 km s$^{-1}$ cloud is evident in neither our lithium data (which have lower S/N ratio than their observations) nor those of MHW. While there is certainly absorption at this velocity in other species (e.g. Welty et al. 1994; Barlow et al. 1995), it should be noted that there are further features, with comparable column densities in Na$^{12}$ and K$^0$, at −12 and −16 km s$^{-1}$, and that a single-cloud fit to LFV’s data leaves both positive and negative residuals of similar amplitude ($\sim 0.04$ per cent of continuum; their fig. 6), possibly as a consequence of very low-amplitude residual fringing in their detector. Furthermore, if the column density of lithium in the −19 km s$^{-1}$ cloud were as large as suggested by LFV, then the implied gas-phase abundance ratio of $\text{Li}^{12}/\text{K}^0$ is $\sim 1.2$ dex − higher by more than 0.5 dex than any sightline in the compilations by Steigman (1996) and Welty & Hobbs (2001).

Irrespective of the lithium column density in the −19 km s$^{-1}$ cloud, the MHW and LFV solutions are essentially indistinguishable in the region of the dominant −15 km s$^{-1}$ blend (and, despite LFV’s criticisms of the MHW fits, yield isotopic ratios that agree to within the joint errors); both agree well with our single-cloud model. We are therefore reassured that the inclusion of any additional components from among the known clouds towards ζ Oph has a negligible influence on the results of modelling the −15 km s$^{-1}$ blend; what is of more interest to our discussion is that this feature is properly analysed.

4.2 UHRF modelling: lithium . . .

The UHRF lithium data can be modelled, independently of all other constraints, with an eight-parameter fit: $v$ and $b$ for each of two clouds in the −15 km s$^{-1}$ blend, together with $N$ for each species in each cloud. We could allow different $b$ values for each
Table 1. Summary of model fits to UHFR data, discussed fully in Section 4. Quoted velocities are heliocentric, and their errors are purely internal, taking no account of possible global zero-point errors (which are considered unlikely to exceed a few tenths of a km s\(^{-1}\)). Column densities for potassium are the sum of \(^{39}\)K and \(^{41}\)K (in the assumed ratio 1:13.9). Error estimates are 68 per cent single-parameter confidence limits from Monte Carlo simulations. The final column gives the percentage of Monte Carlo simulations that yield lithium isotope ratios equal to or greater (less) than the solar-system value, for least-squares solutions that are less (greater) than that value. Model Li–1 is a single-cloud fit to the \(6769\) complex, for comparison with previous analyses. Models Li–2A and 2B are two-cloud fits to the −15 km s\(^{-1}\) blend, with and without the isotope ratios as free parameters. Model K–5 is the multicomponent fit to \(6769\), and models LiK–5A and 5B are simultaneous fits to both Li and K data (again, with and without the lithium isotope ratios as free parameters). The LiKNa  model is a simultaneous fit including the Na \(A3302\) doublet, with the sodium b values and columns given in square brackets; model LiKNa’ has b values constrained to be the same for all species. Our recommended solution is model LiKNa.

<table>
<thead>
<tr>
<th>Model</th>
<th>(v) (km s(^{-1}))</th>
<th>(b(\text{K}^0\text{[Na}^+])) (km s(^{-1}))</th>
<th>(b(\text{Li}^0)) (km s(^{-1}))</th>
<th>(\log_{10}N(\text{K}^0\text{[Na}^+])) (dex cm(^{-2}))</th>
<th>(\log_{10}N(\text{Li}^0)) (dex cm(^{-2}))</th>
<th>(\log_{10}(\text{Li}^0/\text{Na}^+))</th>
<th>(P) (per cent)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Li–1</td>
<td>−14.67 ± 0.23</td>
<td>1.32 ± 0.04</td>
<td>9.541 ± 0.010</td>
<td>8.45 ± 0.10</td>
<td>1.09 ± 0.12</td>
<td>48</td>
<td></td>
</tr>
<tr>
<td>Li–2A</td>
<td>−13.95 ± 0.04</td>
<td>1.17 ± 0.06</td>
<td>9.097 ± 0.011</td>
<td>6.51 ± 0.67</td>
<td>2.59 ± 0.81</td>
<td>2.2</td>
<td></td>
</tr>
<tr>
<td></td>
<td>−14.983 ± 0.027</td>
<td>1.07 ± 0.03</td>
<td>9.346 ± 0.010</td>
<td>8.427 ± 0.048</td>
<td>0.92 ± 0.03</td>
<td>1.8</td>
<td></td>
</tr>
<tr>
<td>Li–2B</td>
<td>−13.93 ± 0.18</td>
<td>1.2 ± 0.17</td>
<td>9.09 ± 0.06</td>
<td>8.00</td>
<td>1.09</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>−14.99 ± 0.26</td>
<td>1.06 ± 0.14</td>
<td>9.35 ± 0.11</td>
<td>8.26</td>
<td>1.09</td>
<td></td>
<td></td>
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<tr>
<td>K–5</td>
<td>−12.91 ± 0.20</td>
<td>0.93 ± 0.35</td>
<td>10.32 ± 0.14</td>
<td></td>
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</tr>
<tr>
<td>LiK–5A</td>
<td>−13.95 ± 0.01</td>
<td>1.1 ± 0.12</td>
<td>9.092 ± 0.007</td>
<td>5.59 ± 0.20</td>
<td>3.50 ± 0.41</td>
<td>4.0</td>
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</tr>
<tr>
<td>LiK–5B</td>
<td>−13.90 ± 0.04</td>
<td>1.07 ± 0.06</td>
<td>9.349 ± 0.010</td>
<td>8.423 ± 0.086</td>
<td>0.93 ± 0.17</td>
<td>3.2</td>
<td></td>
</tr>
<tr>
<td>LiKNa</td>
<td>−13.95 ± 0.01</td>
<td>1.19 ± 0.21</td>
<td>9.08 ± 0.022</td>
<td>7.99</td>
<td>1.09</td>
<td></td>
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</tr>
<tr>
<td>LiKNa</td>
<td>−13.90 ± 0.02</td>
<td>1.07 ± 0.12</td>
<td>9.36 ± 0.007</td>
<td>8.27</td>
<td>1.09</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>−13.95 ± 0.08</td>
<td>1.18 ± 0.21</td>
<td>9.09 ± 0.012</td>
<td>4.7 ± 0.15</td>
<td>4.4 ± 0.4</td>
<td>13</td>
<td></td>
</tr>
<tr>
<td></td>
<td>−14.983 ± 0.08</td>
<td>1.072 ± 0.068</td>
<td>9.351 ± 0.052</td>
<td>8.42 ± 0.13</td>
<td>0.93 ± 0.15</td>
<td>6.1</td>
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<td></td>
<td>−14.983 ± 0.06</td>
<td>0.925 ± 0.90</td>
<td>10.323 ± 0.027</td>
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<td></td>
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</tr>
<tr>
<td>LiKNa</td>
<td>−13.95 ± 0.01</td>
<td>1.2 ± 0.17</td>
<td>10.32 ± 0.19</td>
<td></td>
<td></td>
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<td></td>
</tr>
<tr>
<td>LiKNa</td>
<td>−13.90 ± 0.02</td>
<td>1.2 ± 0.17</td>
<td>10.32 ± 0.21</td>
<td></td>
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</tr>
</tbody>
</table>

isotope, but for purely thermal broadening the values would differ by only 8 per cent (less if any non-thermal broadening is present), and the present data are inadequate to provide discrimination at this level. Furthermore, in principle we should model each separate observation simultaneously (for example, formally to optimize, rather than simply to measure, velocity offsets between them). In practice, however, the S/N ratio in individual observations is such that the statistical ‘best fit’ is often physically unacceptable, as the
software locks on to noise features rather than interstellar lines. We therefore simply model the summed spectra (for which the relative wavelength scales are, in any case, good to fractions of a pixel).

Results for the eight-parameter, lithium-only model are given in Table 1 (Model Li–2A). This fit is formally good, in the sense that the null hypothesis of compatible residuals in the line and in the continuum cannot be rejected. However, the two components contributing to the $-15 \text{ km s}^{-1}$ blend are not resolved (not because of instrumental shortcomings, but because the intrinsic line widths are comparable with the separation), consequently there is a correlation between the line width, the line location and the line strength for each component (while conserving these quantities for the blend). We address this point further in Section 5.1.1.

The most interesting result from the two-cloud fit is that the distributions of solutions from 1000 Monte Carlo replications for the lithium isotope ratios are quite strongly peaked away from the meteoritic value, as indicated by the final two columns of Table 1. Although it should be noted that the final column gives the one-tailed probability that the observed value is consistent with the solar-system value (so that the probability that the two values are the same is twice the tabulated statistic), the $\sim 2\sigma$ differences between inferred and meteoritic isotope ratios clearly merit further investigation.

As a point of reference, we therefore conduct a second two-component fit to the lithium data, in which the isotopic ratio is held fixed at the solar-system value in both clouds (Model Li–2B in Table 1). The resulting model is almost identical to Li–2A, differing by less than 0.0003 continuum units at all wavelengths (that is, expressed in terms of the data errors, by less than 0.4\sigma). Increasing the number of degrees of freedom by two incurs an increase of $\sim 10$ per cent in $\chi^2$, but with $F(2,82) = 0.5$ the two models are, statistically, completely indistinguishable. In other words, the present analysis is consistent with a solar-system lithium isotope ratio in both components of the $-15 \text{ km s}^{-1}$ blend.

### 4.3 Potassium

As noted above, the lithium data alone do not reliably fix the velocity separation of the two clouds contributing to the $-15 \text{ km s}^{-1}$ blend. We therefore look to other absorption-line systems for additional constraints. While it is difficult to be certain that any blend. We therefore look to other absorption-line systems for additional constraints imposed by observations of the D lines. We have also obtained a substantially improved fit, albeit by neglecting additional constraints imposed by observations of the D lines. Barlow et al. discuss the possibility of a third component in the $-15 \text{ km s}^{-1}$ blend, which appears to be required if a satisfactory fit is to be achieved with the UV and D doublets simultaneously; obviously, improved data would be useful to address this question.

For the fits reported in Table 1, we used Na data adjusted in intensity zero-level as described by Barlow et al. (1995); using unadjusted data decreases log N by $\sim 0.1$ dex and increases $b$ by $\sim 5$ per cent, leaving all other parameters virtually unchanged. The lithium isotope ratio is again consistent with meteoritic values (confirmed by an untabulated model in which the ratio is fixed).

Like lithium, potassium has two relatively abundant isotopes, $^{39}\text{K}$ and $^{41}\text{K}$, each displaying hyperfine structure. Using the measurements of hyperfine structure given by Bendall et al. (1981), we have conducted model fits to the $\lambda 7699$ feature, and find that the isotopic ratio for potassium cannot be determined with any useful degree of accuracy from our data. We therefore fix the $^{41}\text{K}/^{39}\text{K}$ ratio at the solar-system value of 13.9 : 1 (Anders & Grevesse 1989). We are unaware of any reason to expect significant spatial variations in this ratio, and in any case the corollary of the indeterminacy of the ratio from our data is that the model fits to $\lambda 7699$ are insensitive to the assumed $^{41}\text{K}/^{39}\text{K}$ ratio. The best-fitting model to $\lambda 7699$ is summarized in Table 1 (model K–5). The tabulated five-cloud model gives a formally significant improvement over a four-cloud model, and is in excellent agreement with the model presented by Welty & Hobbs (2001).

The next step is to fit simultaneously the Li and K data sets, appropriately weighted, allowing these two species to have different $N$ and $b$ values in each cloud, but requiring them to share the same velocities. As expected, lithium proves to be detected in only the $-15 \text{ km s}^{-1}$ blend (in all other clouds the derived column is less than the error on the column). The final model is presented in Table 1 (Model LiK–5A), and is a formally good fit to the data, in that the $F$-test gives no indication that the null hypothesis of compatible residuals in the lines and in the continuum can be rejected.

The additional constraint provided by the potassium line has rather little effect on the lithium model (in part because, in practice, we ‘worked backwards’ from the potassium fit when optimizing the lithium solution). The inferred lithium isotope ratios are again suggestive of non-meteoritic values, but, as in the case of lithium-only fits, imposing the solar-system isotope ratio results in a very similar model profile (differences $< 0.0003$ continuum units); this is Model LiK–5B in Table 1. The conclusion that our data are consistent with a solar-system lithium isotope ratio is that the two components of the $-15 \text{ km s}^{-1}$ blend is therefore unchanged by the inclusion of constraints from the potassium line.

### 4.4 Sodium

Finally, we include the Na $\lambda 3302$ doublet in the model. Partly because of their low weight, the sodium data leave the Li/K model almost unchanged (cf. the LiK and LiKNa models in Table 1). The main benefit from their inclusion is, therefore, simply to provide a more objective estimate of the sodium columns and velocity dispersions than was achieved by Barlow et al. (1995). We have also obtained a substantially improved fit, albeit by neglecting additional constraints imposed by observations of the D lines. Barlow et al. discuss the possibility of a third component in the $-15 \text{ km s}^{-1}$ blend, which appears to be required if a satisfactory fit is to be achieved with the UV and D doublets simultaneously; obviously, improved data would be useful to address this question.

For the fits reported in Table 1, we used Na data adjusted in intensity zero-level as described by Barlow et al. (1995); using unadjusted data decreases log N by $\sim 0.1$ dex and increases $b$ by $\sim 5$ per cent, leaving all other parameters virtually unchanged. The lithium isotope ratio is again consistent with meteoritic values (confirmed by an untabulated model in which the ratio is fixed).

$^8$ A third isotope, $^{40}\text{K}$, is expected to have a negligible abundance: $^{41}\text{K}^{40}\text{K} \approx 8000$ (Anders & Grevesse 1989).

$^9$ Fits that assume $^{39}\text{K} = ^{41}\text{K}$ and $^{39}\text{K} = 0$ yield models that are indistinguishable from those listed here.
5 DISCUSSION

Overall, the fits provide a posteriori justification for assumption of cospatial distributions of the neutral alkali metals, at least to the extent that satisfactory models are achieved with this assumption. Furthermore, the results are broadly insensitive to detailed assumptions concerning the models; we therefore discuss the results of model LiKNa, the simultaneous solution to all three species (noting where other models give different results).

5.1 Line widths

In general, intrinsic interstellar line widths are governed by thermal and ‘turbulent’ broadening (where it is to be understood that ‘turbulence’ is in reality a fudge factor to accommodate any non-thermal velocities), such that

$$b = \left( \frac{2kT_b}{m} + 2\sigma_t^2 \right)^{1/2}$$

for a Gaussian line-of-sight turbulent velocity distribution with rms dispersion $\sigma_t$, where $k$ is Boltzmann’s constant, $T_b$ is the gas kinetic temperature and $m$ is the mass of the atom. We can therefore undertake estimates of both thermal and turbulent contributions from the observed line widths for three species in each cloud in the $-15\,\text{km\,s}^{-1}$ blend.

5.1.1 Results from unconstrained fits

A simple linear fit to the results of model LiKNa ($b^2$ versus $m^{-1}$, using single-parameter errors from the covariance matrix to estimate weights) yields only upper limits to $\sigma_t$ of $<0.26$ and $<0.32\,\text{km\,s}^{-1}$ (3$\sigma$, $-14.0$ and $-15.0\,\text{km\,s}^{-1}$ clouds, respectively); this implies subsonic turbulence for gas temperatures $>20\,\text{K}$.

The formal gas kinetic temperatures are $500 \pm 130$ and $830 \pm 125\,\text{K}$ ($-14.0$ and $-15.0\,\text{km\,s}^{-1}$ clouds). These values are higher than generally found for the diffuse ISM, and are primarily the result of the $-1\,\text{km\,s}^{-1}$ $b$ values found for lithium. A somewhat lower temperature, $390 \pm 210\,\text{K}$, is obtained for the $-15.0\,\text{km\,s}^{-1}$ cloud if the discrepancy in broad result for Na is ignored (on the basis of the problematical line fits discussed by Barlow et al. 1995). Including the results for Fe$^0$ given by Barlow et al. introduces negligible changes to these results, which are sensitive primarily to the light elements.

There is an obvious potential trade-off between the separation of the two main components in the $-15\,\text{km\,s}^{-1}$ blend and their $b$ values. Because the components are intrinsically unresolved in lithium, the main ‘leverage’ on $b$ comes from the line width, so that if the velocity separation (constrained mainly by the K line) is larger than found here, the inferred line width (and $T_b$ values) would be smaller. There are hints that the separations found for molecular lines are indeed slightly larger than our value (e.g. Lambert et al. 1990), but other neutral atomic species are consistent with our result (e.g. Barlow et al. 1995).

To check this, we worked out solutions to the lithium data with the cloud separation fixed at values in the range $1.00-1.30\,\text{km\,s}^{-1}$. These constrained least-squares solutions give best-fitting $b$ values that are almost constant at $\sim1.0\,\text{km\,s}^{-1}$ for the $-15.0\,\text{km\,s}^{-1}$ cloud, and monotonically decreasing from $\sim1.2$ to $\sim0.5\,\text{km\,s}^{-1}$ with increasing separation in the $-14.0\,\text{km\,s}^{-1}$ cloud. For comparison, Crawford et al. (1994) and Lambert et al. (1990) estimate $b$ values for CH of $0.50$ and $0.44\,\text{km\,s}^{-1}$ ($-14.0\,\text{km\,s}^{-1}$) and $0.58$ and $0.75\,\text{km\,s}^{-1}$ ($-15.0\,\text{km\,s}^{-1}$), while Crawford & Williams (1997) find $0.33$ and $0.91\,\text{km\,s}^{-1}$ for NH; for purely thermal broadening, the lithium lines should be $\sim1.4 \times$ wider – as observed.

5.1.2 Fits with $b$ values constrained

While the foregoing discussion suggests that the line width (and implied high kinetic temperature) is apparently reasonably well established, at least for the $-15.0\,\text{km\,s}^{-1}$ cloud, a determination of the kinetic temperatures from C$^2$ molecules in this sightline indicates $\sim20-30\,\text{K}$, for each of the dominant clouds (Crawford 1997). If the kinetic temperature appropriate to the neutral alkali metals were this low, then the line widths would be dominated by turbulence, with the implication that the line-width analysis has led to incorrect results. We are therefore motivated to investigate the consequences of assuming turbulence-dominated line widths.

To do this, we conduct fits with the $b$ parameter constrained to be the same for each species in a given cloud. An illustrative result for a model with the lithium isotope ratio fixed at the solar-system value is listed in Table 1 (model LiKNa) and shown in Fig. 2. The $b$ values are $0.41 \pm 0.04$ and $0.65 \pm 0.04\,\text{km\,s}^{-1}$ in the $-14.0$ and $-15.0\,\text{km\,s}^{-1}$ clouds (cf. $0.65 \pm 0.08$ and $0.35 \pm 0.07\,\text{km\,s}^{-1}$ estimated for C$^2$).

Fits with $b$ values constrained in this way provide significantly poorer matches to the data, primarily because the ‘shoulders’ of the modelled lines, where they approach the continuum, are too narrow compared with the observed profiles. The $F$ test indicates that the constrained-$b$ fits are worse than those in which the $b$ values are allowed to vary, with $>99.9$ per cent confidence. Either this formal result is misleading (for example, the neutral alkali metals may not be distributed cospatially, as assumed), or the kinetic temperature for the species investigated here is greater than the C$^2$ excitation temperature.

5.2 Li/K ratios

The modelled column densities yield the gas-phase K$^0$/Li$^0$ number ratios directly. The column-weighted ratio in the $-15.0\,\text{km\,s}^{-1}$ blend is $\sim2.27\,\text{dex}$, summed over isotopes, while the values in the individual clouds are $\sim2.30$ ($-14.0\,\text{km\,s}^{-1}$) and $\sim2.25\,\text{dex}$ ($-15.0\,\text{km\,s}^{-1}$, with uncertainties of $-0.1\,\text{dex}$). These values compare well with data compiled by Steigman (1996, averaging 2.43 dex) and by Welty & Hobbs (2001; 2.27 dex, range 1.8–2.5).

Conversion from gas-phase neutral-atom abundance ratios to element abundance ratios requires allowance for unobserved ionic species, and for depletion on to grains. Steigman (1996) discusses these issues, finding that

$$\log_{10}\left(\frac{\text{K/\text{Li}}}{\text{K/\text{Li}}^{\odot}}\right) = -0.55 \pm 0.08$$

in the gas phase, implying $(\text{K/\text{Li}}) = 1.72\,\text{dex}$ by number, in each cloud. This ratio is in good agreement with the solar-system ratio (1.82 $\pm$ 0.05; Anders & Grevesse 1989).

5.3 Li abundance and depletion

If we write the fractional abundance of neutral lithium in the gas phase as

$$F = (\text{Li}^0/\text{Li})_{\text{gas}},$$

the total (gas + dust) interstellar abundance with respect to neutral
hydrogen as

$$A = \frac{N(\text{Li}_0)}{N(\text{H}^0)}.$$ 

and the gas-phase depletion factor as

$$\delta_{\text{Li}} = \frac{N(\text{Li})_{\text{gas}}}{N(\text{Li})_{\text{tot}}}$$

then the observed column-density ratio in the neutral gas is

$$\frac{N(\text{Li}^0)}{N(\text{H}^0)} = F \delta.$$ 

The interstellar neutral-hydrogen column towards ζ Oph is \(\sim 20.8\) dex cm\(^{-2}\) (e.g. Shull & van Steenberg 1985), whence \(N(\text{Li}^0)/N(\text{H}^0) = -11.2\) dex. If we assume a ‘cosmic’ ratio of \(N(\text{Li})/N(\text{H}) = -8.7\) dex (Anders & Grevesse 1989), then \(\log F \delta = -2.5\) (with an uncertainty of \(\sim 0.1\); that is, only one lithium atom in \(\sim 300\) is present as a gas-phase neutral atom in the ζ Oph sightline, the remainder being ionized, incorporated into grains or both.

Any estimate of absolute lithium abundances is therefore highly uncertain, because the corrections for unobserved components are both large and sensitive to local conditions. Encouraged by our referee, however, we compare our value for \(\log F \delta\) with estimates of \(F\) obtained from simple ionization-balance calculations:

$$F^{-1} = \frac{\text{Li}}{(\text{Li}^0)_{\text{gas}}} = \frac{\Gamma(\text{Li}^0)}{\alpha(\text{Li}^+)} n_e.$$  \hspace{1cm} (1)

where \(\Gamma(\text{Li}^0)\) is the photoionization rate for \(\text{Li}^0\) and \(\alpha(\text{Li}^+)\) is the radiative recombination rate for \(\text{Li}^+\). The electron density in the line-forming region, \(n_e\) (assumed to be constant), may in principle be estimated from the ratio of column densities for neutral and first (dominant) ionization stages of an appropriate element, by application of equation (1), \textit{mutatis mutandis}, to that element, but suitable observations do not exist with the resolution required to provide values for each of the two dominant clouds. Furthermore, the photoionization rates \(\Gamma\) are liable to depend on the distances of the clouds from ζ Oph. These factors exacerbate already large uncertainties in \(F\) values derived from data summarized by Morton (1975) and by White (1986). (The major source of the difference between these authors is in their inferred electron densities. Both authors adopted similar atomic data, and similar ionization rates, each based on a \textit{mean} diffuse radiation field. If the ionizing radiation field is enhanced by proximity to ζ Oph, then the ratio Li/Li\(^+\) is increased.)

Morton’s data yield \(F^{-1} = 30\) for the integrated column in the \(-15\) \(\text{km s}^{-1}\) blend. Since \(\delta\) must be \(\lesssim 1\), if \(\log F \delta = -2.5\) then Morton’s estimate of \(n_e = 0.7\) \(\text{cm}^{-3}\) must be too large, his adopted
value for the photoionization rate must be too small, the lithium abundance in this sightline must exceed the solar-system value (by at least an order of magnitude), or some combination of these factors must apply. Perhaps more plausibly, White’s estimate of $n_e = 0.1 \text{ cm}^{-3}$ implies $F^{-1} = 380$, hence $\delta = 0.8$ for a solar-system lithium abundance— that is, little or no depletion of lithium from the gas phase.

5.4 $^7\text{Li}/^6\text{Li}$ ratios

The column-weighted average isotopic ratio for lithium is insensitive to details of the cloud model (as one might expect since the lines are very optically thin), with $^7\text{Li}/^6\text{Li} = 1.1 \pm 0.2 \text{ dex}$ for all the solutions presented in Table 1; our adopted solution has $^7\text{Li}/^6\text{Li} = 1.12 \pm 0.2 \text{ dex}$. This value is slightly larger than, but broadly consistent with, the single-cloud results of MHW and LFV, and LFV’s claim that their results are insensitive to unresolved structure is therefore supported to the extent that these average ratios are in agreement. This averaged result is also extremely close to the meteoritic ratio, 1.09 dex (Anders & Grevesse 1989; Chaussidon & Robert 1998), and therefore stands in contrast to LFV’s suggestion that the meteoritic value my be unrepresentative of the ISM value.

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