THE ASTROPHYSICAL JOURNAL, 265:L93–L97, 1983 February 15

EVIDENCE OF NON-LTE IN PHOTOSPHERIC LINES OF G AND K GIANTS

JEFFERY A. BROWN, JOCELYN TOMKIN, AND DAVID L. LAMBERT
Department of Astronomy, University of Texas at Austin
Received 1982 October 1; accepted 1982 October 21

ABSTRACT

A local thermodynamic equilibrium (LTE) model atmosphere analysis of weak Zr I and Ti I lines in 33 field G and K giants suggests that, on the average, Zr is 0.4 dex less abundant relative to Ti than it is in the Sun. The fact that Zr and Ti abundances based on Zr II and Ti II lines do not show any relative overabundance of Zr shows that this Zr underabundance is not real; rather it is strong evidence that some lines of neutral metal atoms are subject to significant departures from LTE. The departures from LTE are more pronounced for the Zr I lines than for the Ti I lines. The nearly identical ionization potentials of Zr and Ti and the similarity of the excitation potentials of the Zr and Ti lines rule out alternative explanations of the spurious Zr underabundance, such as poor choice of the stellar temperatures and gravities or errors in the model atmospheres.

Subject headings: stars: abundances — stars: atmospheres

I. INTRODUCTION

Often, challenging astrophysical questions may be answered by obtaining a key abundance ratio of a pair of similar elements X and Y, where X carries the astrophysical information and Y is the control. Through a careful selection of this control, the abundance ratio X/Y may be quite insensitive to the adopted stellar temperature and surface gravity. Two well-known examples are the combination of the Li I 6707 Å resonance doublet with Ca I lines to provide the Li/Ca ratio (Herbig 1965) and the determination of the s-process enrichment in a red giant's atmosphere from Zr I and Ti I lines and the Zr/Ti ratio (Boesgaard 1970).

In this *Letter*, we point out that departures from local thermodynamic equilibrium (LTE) may invalidate most obvious selections of line pairings intended to provide accurate abundance ratios for red giants. Our conclusion, which follows from an attempt to define the dispersion in the Zr/Ti ratio for a sample of G and K giants, is compatible with the results of a detailed analysis of the bright K0 III giant Pollux (β Gem) by Ruland *et al.* (1980*a*).

II. OBSERVATIONS AND ANALYSIS

Our original program was to determine the ratio of the abundances of zirconium and titanium, extending the earlier study of Boesgaard (1970) to warmer, normal field giants. Our purpose was to determine if a measurable "cosmic dispersion" in s-process abundances exists, as has been suggested by Sneden, Lambert, and Pilachowski (1981) as an explanation of the mild barium stars.

We obtained spectra of 33 giants with the McDonald Observatory's 2.7 m telescope, an echelle grating, and a Reticon self-scanned silicon photodiode array (Vogt, Tull, and Kelton 1978) mounted on the coudé spectrometer. Four wavelength intervals with central wavelengths 4744 Å, 6141 Å, 6266 Å, and 6304 Å containing the lines of Ti I and Zr I listed in Table 1 were observed. Each observation covered about 20 Å of spectrum with a resolution of 0.07 Å (for the λ4744 region) or 0.097 Å (for the other spectra). Interference by telluric lines was minimized by taking the spectra at times when the stellar features were Doppler-shifted away from telluric lines. Signal-to-noise ratios were typically 350 to 1. Continuum placement is not a problem in the selected regions.

The oscillator strengths for most of these lines are based on solar equivalent widths from the Liège solar atlas (Delbouille, Neven, and Roland 1973) and employing a line analysis program, LINES, (Sneden 1973) with the Holweger-Müller (1974) solar model atmosphere. For one Ti line and one Zr line, the solar equivalent widths were unmeasurably small. For these cases, we computed stellar (ε Vir for the Ti I lines, β Gem for Zr I) gf-values from model atmospheres (Bell *et al.* 1976). Solar gf-values for the two weak lines were then computed by scaling the stellar to the solar gf-values. The parameters (5000, 3.0, 0.0) and (4750, 3.0, 0.0) were used for ε Vir and β Gem respectively. [The notation ($T_{\rm eff}$, log g, [M/H]) is used.] The microturbulence was set to 1.7 km s^{-1} in both cases. The quantity log $gf\varepsilon_0$ is given in Table 1, where ε_0 is the elemental abundance relative to hydrogen.

TABLE 1

PROGRAM LINES

Species	λ (Å)	χ (eV)	$W_\lambda(\odot)$ (mÅ)	$\log gf\epsilon_0$	CN Blends
Zr I	4739.45	0.64	5.8	−9.33	none
Zr I	6134.57	0.00	2.6	−10.57	9,4 R_2 8 6134.57
Zr I	6140.46	0.51	0.9	−10.58	8,3 R_2 43 6140.49
Zr I	6143.18	0.07	2.2	−10.55	8,3 P_2 32 6143.12; 9,4 R_2 14 6143.22
Zr I	6304.32	0.54	...	−10.36	none; see text
Ti I	6266.02	1.75	1.1	−9.05	none
Ti I	6273.39	0.02	...	−11.39	none
Ti I	6303.77	1.46	6.9	−8.50	4,0 P2 26 6303.71
Ti I	6312.24	1.44	6.5	−8.55	none

Several of the program lines are blended with weak lines of the CN red system (see Table 1). The lines were deblended by a semiempirical curve-of-growth method (Tomkin and Lambert 1979). The λ6304 line of Zr is unresolved from two CN lines and could only be measured in a few stars. When possible, the unblended half of the profile was measured and the result doubled to obtain the equivalent width.

Temperatures and gravities for the sample stars are given in Table 2. The majority of them are taken from Lambert, Dominy, and Silvertsen (1980); others are from Williams (1971), Tomkin, Luck, and Lambert (1976), and da Silva and Grenier (1977). The effective temperatures are ultimately based on the infrared colors of Johnson *et al.* (1966) and Johnson's (1966) calibration, and the gravities on K line absolute magnitudes (Wilson 1976).

Zirconium and titanium abundances were derived using the equivalent widths, solar *gf*-values, and the LINES program (Sneden 1973). (A list of equivalent widths is available from the authors on request.) Abundances were calculated for each line with model atmospheres from the Bell *et al.* (1976) grid with ($T_{\rm eff}$, $\log g$) values around those of the star. The results for [Ti/H] and [Zr/Ti] relative to the Sun are included in Table 2.

III. DEPARTURES FROM LTE

The Zr/Ti abundance ratio (Table 2) is almost uniformly less than the solar value; the mean is [Zr/Ti] = −0.37. This result can only be accounted for as a signature of departures from LTE affecting both the Ti I and Zr I lines.[1] Other possible sources of systematic error in an LTE abundance analysis may be discounted. An error in the adopted effective temperature has little effect on the Zr/Ti ratio because the ionization potentials of Ti and Zr differ by just 0.02 eV and the mean excitation potentials of the line samples are fairly similar ($\langle\chi\rangle_{\rm Ti}$ = 1.16 eV, $\langle\chi\rangle_{\rm Zr}$ = 0.35 eV). Of course, the abundances Ti/H and Zr/H are temperature depen-

TABLE 2

ABUNDANCE RATIOS RELATIVE TO THE SUN

Star	$T_{\rm eff}$	$\log g$	[Ti/H]	[Zr/Ti]
δ And	4250	2.2	−0.29	−0.62
α Cas	4550	2.1	−0.34	−0.38
β Cet	4800	2.9	−0.16	−0.24
η Cet	4475	2.5	−0.24	−0.40
γ^1 And	4375	1.7	−0.11	−0.38
α Ari	4450	2.5	−0.42	−0.49
γ Tau	4900	2.8	−0.10	−0.35
δ Tau	4950	2.8	−0.11	−0.28
ε Tau	4950	2.8	−0.02	−0.26
θ^1 Tau	5000	3.0	−0.01	−0.25
κ Gem	4900	3.0	−0.36	−0.24
β Gem	4750	2.8	−0.26	−0.33
β Cnc	4000	1.9	−0.52	−0.40
α Hya	4100	1.9	−0.35	−0.39
α UMa	4700	2.5	−0.18	−0.35
ψ UMa	4500	2.7	−0.38	−0.38
ν UMa	4000	1.8	−0.67	−0.47
ε Vir	4950	2.7	−0.20	−0.13
α Boo	4300	1.6	−0.59	−0.59
ρ Boo	4330	2.2	−0.23	−0.64
β UMi	4000	2.0	−0.51	−0.47
α Ser	4500	2.7	−0.17	−0.45
τ CrB	4750	3.2	−0.20	−0.46
β Her	4860	2.5	−0.40	−0.20
β Oph	4550	2.6	−0.14	−0.07
η Ser	4900	3.0	−0.30	−0.36
η Cyg	4760	2.9	−0.21	−0.26
ε Cyg	4710	2.9	−0.26	−0.44
η Cep	4850	3.5	−0.40	−0.39
ζ Cyg	4875	2.8	−0.32	0.02
ι Cep	4680	2.8	−0.27	−0.35
γ Psc	4775	2.8	−0.65	−0.49
γ Cep	4750	3.3	−0.06	−0.49
Average	...	...	−0.29	−0.37

[1] Helfer and Wallerstein (1968) derived abundances for 27 giants. Examination of their tables appears to show that the [Zr/Ti] ratios are slightly scattered about zero. Since they used an average of three of the Hyades giants and not the Sun as the standard star in their differential abundance analysis, they did not realize that the ratio was smaller than the solar value.

dent. A 500 K increase in T_{eff} for the typical giant changes the Zr/Ti ratio by only +0.16 dex as Ti/H is increased by 0.78 dex. Surface gravity is an even less significant source of error: if $\log g = 2.25$ is increased to $\log g = 4.5$ (a main-sequence star!), Zr/Ti changes by only +0.10 dex and Ti/H by +0.12 dex.

A low Zr/Ti ratio is not attributable to our use of weak lines in the solar spectrum. Although our solar equivalent widths agree well with published measurements (Ruland *et al.* 1980*b*; Biémont *et al.* 1981), we must consider the possibility that some of these weak solar lines may be contaminated by unidentified blends. As a check, we recomputed the stellar abundances from reference solar abundances and the accurate laboratory oscillator strengths available for four Zr I lines (Biémont *et al.*) and two Ti I lines (Whaling, Scalo, and Testerman 1977). Reference abundances—$\log \varepsilon(\text{Zr}) = 2.60$ and $\log \varepsilon(\text{Ti}) = 4.95$—were taken from a new table of solar system abundances (Anders and Ebihara 1982) which is compiled from analyses of C1 meteorites with normalization to the scale $\log \varepsilon_{\text{H}} = 12.00$ based on a comparison of solar and meteoritic abundances of nine elements. Of course, the stellar Zr/Ti ratio is here set by the meteoritic Zr/Ti ratio and is independent of the normalization factor. Anders and Ebihara emphasize that meteoritic and photospheric abundances of nonvolatile elements are in fine agreement for all but two or three elements. This alternate approach changes the mean [Zr/Ti] value of our sample by less than 0.02 dex. It suggests that the systematic errors (blends, non-LTE effects) in [Zr/Ti] arising from our use of solar lines is less than ±0.05 dex. Clearly, our choice of solar lines is not the key to the low [Zr/Ti] values.

Our stellar spectra are of high quality, and comparisons with published equivalent widths show good agreement; for example, the Reticon equivalent widths for β Gem and those published by Ruland *et al.* (1980*b*) are in fine agreement (Tomkin and Lambert 1983). The Ti I and Zr I line selection excludes saturated lines sensitive to the adopted microturbulent velocity. Finally, the line analysis computer program has been checked thoroughly; our results for β Gem match those published by Ruland *et al.* (1980*a*) when their atmosphere, equivalent widths, and the solar oscillator strengths required by their solar equivalent widths (Ruland *et al.* 1980*b*) are used with our program.

For a sample of stars of the same metallicity, abundance ratios such as Zr/Ti must show a cosmic scatter about a mean value. The Sun is possibly unrepresentative of that mean value. Fortunately, Spite (1968) has provided Zr/Ti ratios for 12 unevolved stars. The Zr/Ti ratio declines with decreasing [Ti/H] (Fig. 1), but the best fitting linear relation shows that the Sun is certainly within 0.1 dex of the mean value for solar metallicity dwarfs. (A similar conclusion holds for the [Ba/Ti] versus [Ti/H] relation compiled from Wallerstein's 1962 abundance analysis of about 30

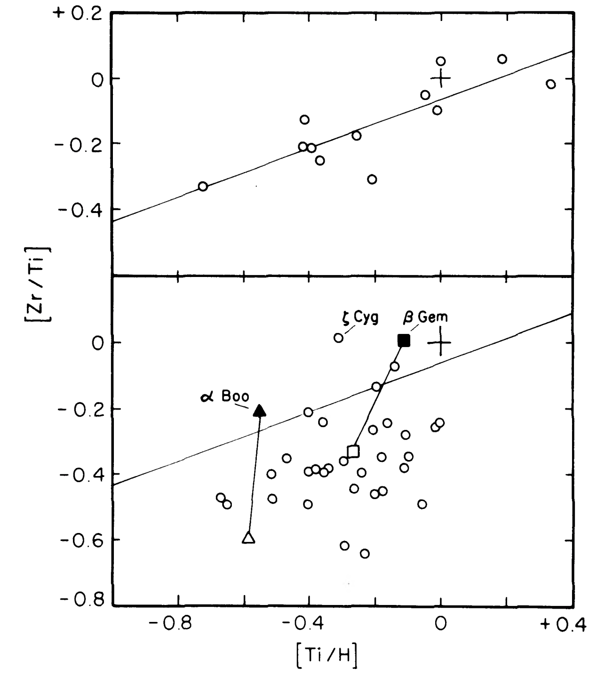

FIG. 1.—(*upper*) Open circles are [Zr/Ti] vs. [Ti/H] for dwarfs from Spite (1968). The line is fitted by eye to the data. The plus sign indicates solar values. (*lower*) Open circles are [Zr/Ti] vs. [Ti/H] for 33 giants of this study. Filled triangles are values based on ionized lines (see text); the line and plus are the same as above.

dwarfs. Of course, the Zr/Ba ratio may evolve with increasing metallicity.) The Zr/Ti results for the giants (Fig. 1, *lower*) are clearly displaced below the mean relation of Spite's sample; the mean vertical displacement is −0.20 when the mild Ba star ζ Cyg, classified G8+ III–IIIa Ba0.6 by Keenan and Pitts (1980), is excluded. The trend to lower Zr/Ti ratios at lower Ti abundances does seem to be reproduced by the giants. It is obvious too that the maximum Ti abundance is lower in the sample of giants. The scatter of the [Zr/Ti] values about the mean is just slightly larger than our estimated measurement errors.

Key evidence that our Zr/Ti ratios are too small comes from the Ti II and Zr II lines. Observations of these lines in β Gem (Ruland *et al.* 1980*a*) and α Boo (Mäckle *et al.* 1975) yield [Zr/Ti] ratios of +0.01 and −0.21 respectively.[2] These ratios are ~0.35 dex larger than our values of −0.33 (β Gem) and −0.59 (α Boo), which are based on neutral lines. In Figure 1, the pairs of points obtained from (Zr I, Ti I) and (Zr II, Ti II) lines are connected by straight lines. Note that the points based on the Zr II and Ti II lines fall close to the relation defined by Spite's (1968) sample. (Use of our

[2]The β Gem result is from Table 6 of Ruland *et al.* and the α Boo result is the average for all Zr II and Ti II lines of Mäckle *et al.* with $\log W/\lambda < -4.7$.

temperatures and gravities for β Gem and α Boo instead of those of Ruland *et al.* 1980*a* and Mäckle *et al.* 1975 would not change the [Zr/Ti] derived from their Zr II and Ti II lines; it would increase the [Ti/H] by 0.1 and 0.2 dex respectively.)

In the atmosphere of a G or K giant, the ions Ti^+ and Zr^+ are the dominant species. A severe reduction in the neutral atom density can produce only a minor increase in the ion density. Then, if "overionization" is the principal manifestation of departures from LTE, the ions will yield in an LTE analysis abundances close to the correct values. There is no LTE analysis of either β Gem or α Boo that can reconcile the Zr/Ti ratios from both the neutral and ionized lines.

IV. CONCLUDING REMARKS

The existence of pronounced departures from LTE was first demonstrated by Ruland *et al.* (1980*a*) for β Gem. They showed that an LTE analysis of iron-peak elements (Ti I, Ti II; Cr I, Cr II; Fe I, Fe II) gave normal (i.e., quasi-solar) abundances from the ionized and high-excitation neutral lines but low abundances from the low-excitation neutral lines; our Ti I and Zr I lines are low-excitation lines by their definitions. Of course, such abundance differences may be reduced or removed by selecting a higher effective temperature. Indeed, the requirement that the elemental abundance be independent of excitation potential is commonly used to determine the effective temperature. Ries (1981) remarks that the iron abundance differences noted by Ruland *et al.* may be eliminated by adoption of a higher effective temperature. (Ionization equilibrium is restored with a concomitant increase in the surface gravity.) When the resulting effective temperature is tested against the continuous spectrum—for example, the infrared flux method (Blackwell and Shallis 1977)—suspicions arise because the temperatures appear to be too hot (Lambert and Ries 1981). Such suspicions are difficult to confirm or to deny. Our LTE determinations of the temperature-insensitive Zr/Ti ratio show beyond reasonable doubt that departures from LTE must vitiate LTE analyses of neutral metal lines. The similarity in the structures of the neutral Ti and Zr atoms probably moderates the influence of departures from LTE on the calculation of the Zr/Ti ratio.

Theoretical studies of the statistical equilibrium of model atoms in red giant atmospheres (and main-sequence stars) are stuck at an elementary level. A pioneering study of Fe I examined a greatly simplified model atom in a very small sample of atmospheres (Lites and Cowley 1974). As Ruland *et al.* (1980*a*) stress, this study may not represent real atoms in real atmospheres. Quantitative definition by observers of the departures from LTE will require thorough analyses. We note that the Ti and Zr abundances show no marked trends with $T_{\rm eff}$ or log g that provide a clue to the key factor responsible for the departures from LTE. Both Ti/H and Zr/H show a small decline with decreasing $T_{\rm eff}$ and log g. This is, in part, attributable to the systematic shift in the giant branch to cooler temperatures with decreasing mass and the fact that the metal-poor stars are on average of lower mass.

Our study of Ti I and Zr I lines in G and K giants provides essentially incontrovertible evidence that departures from LTE affect these (and similar) species. We fully endorse Ruland *et al.*'s (1980*a*) warnings about serious departures from LTE. Ruland *et al.* state that the non-LTE effects are greatest for saturated lines (W_λ = 100–150 mÅ), with the effects being smaller for lines weaker and stronger than this. Only six stars in our program have some lines with equivalent widths greater than 100 mÅ. It seems certain that use of weak, unsaturated lines is not sufficient to avoid these problems of non-LTE.

The astrophysicist seeking accurate abundance data may find that a ratio such as Zr/Ti can be derived with good precision from Zr II and Ti II lines and crude estimates of the atmospheric structure; however, more thorough studies are needed of an ion's excitation equilibrium. Unfortunately, other ratios must be derived from the lines of neutral atoms and, in these cases, an assessment of the departures from LTE is now imperative; the Li abundance obtained from the 6707 Å resonance doublet and calibrated against Ca I or Al I is the outstanding example of this second category of abundance ratios.

We thank J. F. Dominy, J. Scalo, C. Sneden, and B. Twarog for helpful discussions. J. A. B. is pleased to thank the Robert A. Welch Foundation of Houston for a predoctoral fellowship. This research has been supported in part by National Science Foundation grants AST 79-22014 and AST 81-17485.

REFERENCES

Anders, E., and Ebihara, M. 1982, *Geochim. Cosmochim. Acta*, in press.
Bell, R. A., Eriksson, K., Gustafsson, B., and Nordlund, A. 1976, *Astr. Ap. Suppl.*, **23**, 37.
Biémont, E., Grevasse, N., Hannaford, P., and Lowe, R. M. 1981, *Ap. J.*, **248**, 867.
Blackwell, D. E., and Shallis, M. J. 1977, *M.N.R.A.S.*, **180**, 177.
Boesgaard, A. M. 1970, *Ap. J.*, **161**, 163.
da Silva, L., and Grenier, S. 1977, *Astr. Ap. Suppl.*, **29**, 195.
Delbouille, L., Neven, L., and Roland, G. 1973, *Photometric Atlas of the Solar Spectrum from λ3000 to λ10000* (Liège: Institut d'Astrophysique).

Helfer, H. W., and Wallerstein, G. 1968, *Ap. J. Suppl.*, **16**, 1.
Herbig, G. H. 1965, *Ap. J.*, **141**, 588.
Holweger, H., and Müller, E. A. 1974, *Solar Phys.*, **39**, 19.
Johnson, H. L. 1966, *Ann. Rev. Astr. Ap.*, **4**, 193.
Johnson, H. L., Mitchell, R. I., Iriarte, B., and Wisniewski, W. A. 1966, *Comm. Lunar Planet. Lab.*, **4**, 99.
Keenan, P. C., and Pitts, R. E. 1980, *Ap. J. Suppl.*, **42**, 541.
Lambert, D. L., Dominy, J. F., and Silvertsen, S. 1980, *Ap. J.*, **235**, 114.
Lambert, D. L., and Ries, L. M. 1981, *Ap. J.*, **248**, 228.
Lites, B. W., and Cowley, C. R. 1974, *Astr. Ap.*, **31**, 361.
Mäckle, R., Griffin, R., Griffin, R., and Holweger, H. 1975, *Astr. Ap. Suppl.*, **19**, 303.
Ries, L. M. 1981, Ph.D. thesis, University of Texas at Austin.
Ruland, F., Holweger, H., Griffin, R., Griffin, R., and Biehl, D. 1980*a*, *Astr. Ap.*, **92**, 70.
Ruland, F., Holweger, H., Griffin, R., and Biehl, D. 1980*b*. *Astr. Ap. Suppl.*, **42**, 391.
Sneden, C. 1973, Ph.D. thesis, University of Texas at Austin.
Sneden, C., Lambert, D. L., and Pilachowski, C. A. 1981, *Ap. J.*, **247**, 1052.
Spite, M. 1968, *Ann. d'Ap.*, **31**, p. 269.
Tomkin, J., and Lambert, D. L. 1979, *Ap. J.*, **227**, 209.
______. 1983, *Ap. J.*, submitted.
Tomkin, J., Luck, R. E., and Lambert, D. L. 1976, *Ap. J.*, **210**, 694.
Vogt, S., Tull, R. G., and Kelton, P. 1978, *Appl. Optics*, **17**, 574.
Wallerstein, G. 1962, *Ap. J. Suppl.*, **6**, 407.
Whaling, W., Scalo, J. M., and Testerman, L. 1977, *Ap. J.*, **212**, 581.
Williams, P. M. 1971, *M.N.R.A.S.*, **153**, 171.
Wilson, O. C. 1976, *Ap. J.*, **205**, 823.

Jeffery A. Brown, David L. Lambert, and Jocelyn Tomkin: Department of Astronomy, University of Texas at Austin, Austin, TX 78712