HYPERFINE STRUCTURE IN THE BARIUM RESONANCE LINE: CURVES OF GROWTH FOR SOLAR AND *r*-PROCESS ISOTOPIC MIXTURES

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ABSTRACT

Equivalent widths of spectral lines of elements with even atomic numbers can be affected by hyperfine structures (hfs) in the isotopes with odd numbers of neutrons. We show that the most commonly studied line of the resonance doublet of barium, λ 4554, is affected by hfs that could change the abundance by some 0.5 dex in unfavorable cases. The relative importance of hfs for this line is greater if the isotopic mix corresponds to the *r*-process. This might be the case in the oldest stars. Only modest changes in the generally accepted historical trend of *r*- to *s*-process abundances are expected when corrections for the hfs are made. Many barium determinations in old stars do not depend on the use of the λ 4554 line. In any event, the errors introduced by neglect of hfs are of the same order as those due to uncertain damping, microturbulence, and non-LTE. We discuss the importance of blends, and the possibility of detecting the *r*-process isotopic mixture—the latter prospect is not good.

Subject headings: atomic processes — stars: abundances — stars: Ba II — Sun: spectra

I. INTRODUCTION

Hyperfine structure (hfs) is usually neglected in stellar abundance work. Nevertheless, it is known to be of importance for certain transitions. A pioneering study by Abt (1951) showed that the hfs widths of lines of several species of atomic spectra were clearly noticeable on the Utrecht Atlas as well as in solar spectra obtained at Mount Wilson. Unsöld's (1955) classic text discussed hfs and pointed out that it could be approximately included in line strength calculations by adding a term to the Doppler width. Unsöld stressed that the hfs widths of some lines were of the order of tenths of angstroms and must not be neglected, but he noted such broadening is generally unimportant for elements with even Z. While this is typically true, we shall show here that nonnegligible effects due to hfs can also occur in some lines belonging to even-Z elements. This structure should be routinely taken into account in future abundance work.

Hyperfine structure arises from the interaction of nuclear spin with the atomic electrons. If Z is odd, a nucleus has an unpaired nucleon, and therefore a net spin. Consequently, hfs is expected for such elements, and broad patterns are known in V I, Mn I, Pr II, Eu II, etc. Heavy elements with even Z have typically five to seven stable or long-lived isotopes; tin has 10. Among these, the isotopes with even N are typically more abundant than those with odd N, and only the latter have an unpaired nucleon and a nonzero spin. The isotopic abundances of individual odd-N nuclides of an even-Z element are rarely as much as 10% of the total species. There are several important exceptions to this, one of which is the element barium.

We examine here the resonance line of Ba II, $\lambda 4554$, whose equivalent width in solar-type stars falls at the strong end of the "flat part" of the curve of growth; at this location, the effect of hfs on the line strength is relatively minor (see below). The second component of the ${}^{2}S{}^{-2}P$ resonance doublet containing $\lambda 4554$ is $\lambda 4934$. It is closely blended with an Fe I line, and therefore less useful for abundance purposes. We shall make some general comments on blends in § IV. Many stellar abundances are based on subordinate Ba II lines whose hfs widths are smaller than λ 4554. These lines are not without difficulties of their own. In many stars, the equivalent widths are sensitive to the assumed microturbulent parameter, and as we shall see, some are blended. An astronomer would be ill-advised to neglect entirely the information available from λ 4554, or a carefully synthesized λ 4934. Abundances determined from subordinate Ba II lines which differed *greatly* from those determined using $\lambda\lambda$ 4554 and 4934 would be suspect. Further, if these lines can be computed accurately, they can help to determine the microturbulent velocities, and thus strengthen the abundance determinations for other species.

Holweger and Müller (1974) determined the solar abundance of barium, and discussed hfs in the Ba II line $\lambda 4554$, showing that it gave rise to noticeable effects both in the profile and the equivalent width. They also included hfs in calculations of subordinate Ba II lines and showed its effect was relatively unimportant. Their paper does not address the general problem of the influence of hfs on stellar barium or other even-Z elemental abundances, the focus of the present work.

Holweger and Müller also discussed departures from LTE in several of the barium lines. These departures typically manifest themselves by deeper line cores than are calculated with the LTE code. It should be mentioned that the temperature distribution in the highest layers of the Holweger-Müller model is chosen to fit the cores of "average" strong lines, but it has been known since Holweger's (1967) dissertation work that this was at best a useful compromise. In this study, we will not consider departures from LTE; the hfs is relevant to any calculation, whether done in LTE or non-LTE.

Very recent stellar abundance work by Magain (1989) has included hfs in the Ba II λ 4554 line. His results will be discussed in § V.

An intriguing aspect of hfs in barium has recently become relevant. Evidence has accumulated that the ratio of the r- to s-process contribution to heavy elements, including barium, is

TABLE 1

FRACTIONAL	ISOTOPIC	ABUNDANCES OF	
	BARIUM	ε.	

1					
A	Sun	Solar r-Process			
130	0.0064	0.0			
132	0.0064	0.0			
134	0.027	0.0			
135	0.0652	0.373			
136	0.074	0.0			
137	0.112	0.143			
138	0.709	0.483			

greater among the extreme metal-poor stars (see Gilroy *et al.* 1988, and § V below). If this is indeed correct, then in the most metal-poor stars, the odd-N nuclides of barium will become relatively more abundant. This is shown in Table 1, where we list the relative abundances (percent by number) of barium isotopes in the "Sun," and in the *r*-process contribution, according to Käppeler *et al.* (1982). Due to shielding, and the shift of the N = 82 *r*-process peak toward lighter nuclides, the two odd-N isotopes actually make up the majority of the *r*-process contribution. By contrast, the solar abundances are dominated by the neutron magic ¹³⁸Ba.

We would thus expect hfs to be much more important in those stars born early in the history of the Galaxy (see below).

II. CALCULATION OF HYPERFINE STRUCTURE PATTERNS

Hyperfine "multiplets" are discussed in numerous texts on atomic structure (cf. Cowan 1981). The splitting of the levels must be obtained from experiment, or a rather sophisticated calculation. Many of the important hfs measurements of astrophysical interest are decades old. Becker and Werth (1983) give a relatively recent measurement of the hyperfine splitting of the $6S_{1/2}$ and $6P_{1/2}$ levels in ¹³⁵Ba, while Blatt and Werth (1982) give similar information for ¹³⁷Ba. These values do not differ significantly from those given by Brix and Kopferman (1952), which we have adopted here, since the latter also give relevant values for the ² $P_{3/2}$, not available in the newer sources.

Nuclear volume effects, also known as isotope shifts, are discussed by Condon and Shortley (1951), and more recently by Cowan. They apply to both odd- as well as even-A isotopes. The shifts are occasionally very large, as in the case of Hg II λ 3984 or Pt II λ 4046 (cf. Dworetsky, Storey, and Jacobs 1984; Engleman 1989). Shifts for Ba II λ 4554 have been taken from Arroe (1950). The maximum shift, for ¹³⁸Ba II–¹³⁰Ba II, is only 0.0044 Å. We have not attempted to account for such higher order effects as the J-dependence of isotope shifts.

The compilations of the US National Bureau of Standards (cf. Musgrove and Zalubas 1989) include papers on hfs and isotope shifts. Heilig (see Heilig 1987) has compiled several bibliographies of isotope shifts.

In contrast to the widths, relative *intensities* of hfs components are easily calculated. The LS-coupling ratios (cf. Condon and Shortley 1951, Table 1⁹) may be used with the transformation $L \rightarrow J$, $J \rightarrow F$, $S \rightarrow I$, in standard notation. If we normalize in such a way that the sum of the strengths of all of the lines in the hfs multiplet is unity, then the strength of the individual lines are given by

$$S(\gamma JIF, \gamma' J'IF') = \frac{(2F+1)(2F'+1)}{(2I+1)} W^2(J'JF'F, 1I), \quad (1)$$

where the W is a Racah coefficient. Rose (1957; see Table I.4)

gives nine equations for W(a, b, c, d; 1f) that are easily adapted for machine computation; Zare (1988) has published FORTRAN programs for calculation of the equivalent 6-*j* symbols.

The S values from equation (1) will be the same as those obtained by adding the tabular entries for all the lines of a multiplet from Condon and Shortley's Table 1⁹ and dividing each of the entries by that sum. The normalized intensities for the λ 4554 hyperfine components are shown in Table 2. The total angular momentum quantum number F is given for the upper (u) and lower (l) levels. Note that the spin of both odd-N barium isotopes is 3/2.

In our calculation for $\lambda 4554$, we have included 17 lines from seven isotopes in the case of the solar isotopic mixture (see Table 1). The *r*-process mixture contains only isotopes with mass numbers 135, 137, and 138, and the number of lines was 13. Our synthesis code (see below) does not include *explicit* provisions for hfs, but it is readily incorporated. We made calculations for 17 or 13 Ba II lines, as appropriate, all with the excitation potentials for $\lambda 4554$. The individual *gf*-values for each line were multiplied by a product of two factors, ϵ_I and i_{hfs} , which take into account the relative abundances of the isotopic species and the hyperfine intensities (cf. Tables 1 and 2). Both factors are normalized to unity, so that the strength of a weak line is the same as that calculated for a single line with no hfs.

III. THE CURVES OF GROWTH

Several curve-of-growth families were calculated based on the model atmosphere spectral-synthesis codes used by Cowley and his coworkers (cf. Cowley and Greenberg 1988). We used the $T(\tau_{5000})$ from the Harvard-Smithsonian Reference Atmosphere (Gingerich *et al.* 1971) to construct the temperaturepressure structure between $\log(\tau_{5000}) - 4.0$ to +1.2. A metal-poor model was constructed using the $T(\tau_{5000})$ of Kurucz's (1979) tabulation for $T_{\rm eff} = 6000$ K, $\log(g) = 4.0$, and $\log(A) = -2.0$. Details of the models are relatively unimportant in the present study.

The natural broadening of the λ 4554 line is included in our calculations as well as van der Waals and Stark broadening. For the former, we used Unsöld's (1955) relation (82, 55) for C_6 , but multiplied the resulting γ_6 by a factor of 2. Broadening by helium is included. For Stark broadening, we used the formula of Cowley (1971).

The most important source of collisional broadening is van der Waals interactions, and the uncertainty in the C_6 parameter can give rise to computed equivalent width differences that are of the same order as the hfs. The effects of changes in C_6 on computed equivalent widths depend on the line strengths, the microturbulence, and the isotopic mix. A detailed discussion is beyond the scope of the present paper, but we provide a few figures for orientation purposes. They are based on the solar model and isotopic mix with no blends; the assumed micro-

 TABLE 2

 Normalized Hyperfine Intensities for

Ba II λ4554: i _{hfs}							
	F (u)						
F (<i>l</i>)	3	2	1	0			
2	0.438	0.156	0.031				



FIG. 1.—Curves of growth for a solar model atmosphere with and without hfs for a solar isotopic mix, and for two values of the microturbulence, ξ_t . Squares: $\xi_t = 0 \text{ km s}^{-1}$, no hfs splitting; stars: $0 \text{ km s}^{-1} \xi_t = 0$, with hfs; triangles: $\xi_t = 1 \text{ km s}^{-1}$, no hfs; circles: $\xi_t = 1 \text{ km s}^{-1}$ with hfs. Tick marks on ordinate are 1.0 dex apart.

turbulence was 1 km s⁻¹. If we multiply γ_6 by 3.0 rather than 2.0, a 69 mÅ line becomes 71 mÅ, a 127 mÅ line becomes 138 mÅ, while a 278 mÅ line becomes 323 mÅ.

The results of the calculations using twice Unsöld's γ_6 are shown in Figures 1 and 2. The abscissae are logarithms of the ratio of the elemental abundance of barium to the sum of all of the elemental abundances. Four curves of growth are shown with and without hyperfine structure for assumed microturbulences of 0 and 1 km s⁻¹. It is readily seen that with a "solar" isotopic mix, the hfs simulates a microturbulence of about 1 km s⁻¹. The solar equivalent width of λ 4554 is 189 mÅ [log (W) = 2.28], according to Holweger and Müller (1974); one can see that the overall effect of the hfs is only a few percent for lines of this strength. The maximum effect will be for lines between about 50 and 100 mÅ.

Figure 2 shows the larger effects from a pure *r*-process mixture of barium isotopes. Errors of a factor of 3 can be made





in unfavorable cases. The "sensitive" range of equivalent widths is some 25–100 mÅ.

Stars with equivalent widths in this range occur among mid-A's to mid-F's with solar abundances. Many CP (Ap and Am) stars have equivalent widths in this range (see Adelman 1973; Sadakane and Nishimura 1979). Barium is typically—though not always—weak in magnetic CP stars, and allowance for hfs in the analyses would exaggerate a trend that is already recognized. The hfs has roughly the same effect as a micro-turbulence of 1 km s⁻¹, so its effect on equivalent widths is about the same as that of a surface field of 1 kG.

Cooler stars can also have λ 4554 equivalent widths in this range if they are metal-poor. We consider the latter stars in the next section.

IV. FAINT BLENDS

According to Moore, Minnaert, and Houtgast (1966), Ba II λ 4554 is flanked by two weak, unidentified features at $\lambda\lambda$ 4553.838 and 4554.252. Such a line would be traditionally considered "unblended." However, largely as a result of the work of Kurucz (cf. Kurucz 1988), there now exists a much larger atomic data base to draw on than was available to Moore, Minnaert, and Houtgast, and we have made a search to see if any of the new information changes the "unblended" nature of λ 4554 (see Table 3 below).

With the help of a data tape kindly made available by Dr. Kurucz, rough, predicted intensities were calculated for T = 5040 K, log $(P_e) = 1.5$, and solar abundances. The overall method is described by Cowley and Merritt (1987). The intensity parameters which appear in Table 3 are equivalent to curve of growth abscissae in a slab or Schuster-Schwarzschild model. Johansson and Cowley (1988) refer to lines that became known after the Multiplet Tables were compiled as "second-generation lines." We found no such lines near $\lambda 4554$. We investigated two weak lines, $\lambda 4553.949$ of Cr I, and $\lambda 4553.96$ of Zr II, which *are* in the Multiplet Tables. The relative importance of these two lines on the overall equivalent width of the Ba II feature may be determined. For the former line, we took the Kurucz (1988) gf-value of -0.81. For Zr II, the interpolation formula of Cowley and Corliss (1983) gives -0.57.

We calculated curves of growth for the $\lambda 4554$ feature including both perturbers, assuming the abundances of all three elements varied in lockstep. If we increase both *gf*-values by 0.5 dex, nonnegligible increases in the calculated equivalent widths occur. The variation depends on the hfs and its isotopic mix as well as the assumed microturbulence, so we give only some

TABLE 3

PARTIAL LIST OF BLENDS WITH BA II LINES							
Spectrum	λ	$E_l ({\rm cm}^{-1})$	Intensity Parameter	Generation			
Ba II	4130.66	21952.422	0.66	1			
Co I	4130.520	4142.66	0.46	1			
Ван	4524.93	20261.562	- 2.29	1			
Тіт	4524.946	19421.576	- 1.48	2			
Ba 11	4554.03	0.0	1.74	1			
Cr 1	4553.945	33040.100	-0.98	1			
Zr 11	4553.97	19514.84	-2.05	1			
Ва II	5853.68	4873.850	-0.09 - 0.51	1			
Fe I	5853.682	33801.567		2			
Ва II	6141.72	5674.824	0.80	1			
Fe i	6141.730	29056.321	0.69	1			

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representative figures, based on $\xi_t = 0.0$ and no hfs. Without the perturbers, calculated equivalent widths along a curve of growth for the solar model were 29, 59, 144, and 421 mÅ. With the perturbers included along, and using enhanced *gf*-values, the corresponding figures were 29, 61, 151, and 447 mÅ. These weak lines *should* be included in future syntheses of the λ 4554 feature, but for the present, we note that they introduce uncertainties smaller than those due to the microturbulence and collisional broadening.

In the course of our search for blends with the λ 4554 line, we examined the regions near other Ba II lines that have been used in the past in abundance studies. While it is beyond the scope of the present paper to comment in detail on the effects of these blends, we list some of them in Table 3 to give the reader a sense of the relative importance of these blends. *The list is not intended to be complete*. Note that the intensity parameters are logarithmic. It appears that at least some published abundances for barium ought to be corrected for blends. Second-generation lines are indicated by a 2 in the last column of the table. The Ba II line λ 6496.90 has no close blends that we could find.

Two of the lines in Table 3 appear among the recent critically evaluated transition probabilities by the workers at the National Bureau of Standards. For Cr I λ 4554.94, Martin, Fuhr, and Wiese (1988) give $\log (gf) = -0.73$, with an "accuracy" of D (within 50%). For Fe I λ 6141.73, Fuhr, Martin, and Wiese (1988) give -1.61, with an accuracy of C (within 25%). The recent Kurucz log (gf) values were -0.81 and -1.54 respectively, within the accuracy estimates of the Bureau of Standards workers.

V. DISCUSSION

Many barium abundance determinations are independent of hfs in $\lambda 4554$, either because the line was not used at all or because the strengths of the lines are unaffected by hfs. For example, neither the studies of Pilachowski, Wallerstein, and Leep (1980) nor Spite *et al.* (1987) used $\lambda 4554$. While Luck and Bond (1981) *did* use this line, their results show no obvious trend that might be attributed to hfs.

Perhaps the influence of hfs is evident in the work of Magain (1985). He measured equivalent widths for λ 4554 of 18 and 58 mÅ in the classical subdwarfs HD 140283 and HD 19445, respectively. In this study, the barium abundances were based only on λ 4554, and we would expect the abundance of barium in HD 19445 is artificially enhanced by the neglect of hfs. This could explain why the last point (Ba) for HD 19445 in his Figure 10 fails to parallel that for HD 140283. A calculation using our "metal-poor" model shows that the enhancement due to hfs is 0.14 and 0.26 dex depending on whether the solar or *r*-process isotopic mix is used.

Magain's (1989) study of abundances in 20 halo dwarfs was received a few days prior to submission of the present paper. In the new work, hfs in the Ba II λ 4554 line is taken into account following the Kiel dissertation work of Biehl (1976). The new study shows [Ba/Fe] = -0.09 which should be compared with -0.05 of the 1985 paper. The small difference in the two results, one with and one without hfs, may be due to the damping. The former work used enhancements of γ_6 of a factor of 1.5, while the more recent work uses a factor of 3, following Holweger and Müller (1974). We suggest the enhancement of a factor of 3 may be too large. The recent study does not discuss the possibility of a nonsolar isotopic ratio. Peterson (1976) also used only λ 4554. Her Figure 3 is a graph of [M/Fe] versus [Fe/H]. The highest points on this plot are for barium in the stars HD 94028 and HD 108177 for which the equivalent widths of λ 4554 were 122 and 80 mÅ, respectively. The points are arguably 0.3–0.5 dex "too high" judging simply from the positions of the other points on the graph. At least part of this discord is reasonably attributed to the microturbulent velocity used, 0.5 km s⁻¹, for the plotted abundances. For HD 94028, Peterson's Table 2 gives calculations based on $v_t = 0.5$ and 1.0 km s⁻¹, and the difference in the barium abundance is about 0.1 dex. If another 0.2 dex could be attributed to hfs, the barium point for HD 94028 would move downward, into the group of five points above which it now lies.

In addition to the uncertainties in abundances derived from λ 4554 that arise from hfs and microturbulence, additional errors can arise from the very poorly known van der Walls broadening. Little work has been done to improve the accuracy of collisional broadening of metal lines by neutral hydrogen for several decades.

The papers cited above, along with similar work, are generally taken as evidence that the ratio of s- to r-process nuclides was lower at the time the extreme metal-poor stars formed than it is today (cf. Spite and Spite 1985; Andreani, Vangioni-Flam, and Audoze 1988). The result is perhaps not new (cf. Wallerstein *et al.* 1963), but it has only recently become widely accepted (cf. Butcher 1975).

We do not expect inclusion of hyperfine structure in $\lambda 4554$ to impact in a fundamental way on the general notion of an increase in the ratio of *s*- to *r*-process nuclides as a function of time. As stellar abundances are refined, it may be that some of the "abruptness" with which the *s*-process appears to have turned on may be lost. This abruptness could at least in part be due to a spurious enhancement in the barium abundances of stars with [Fe/H] about -2.0 where equivalent widths reach a maximum sensitivity to hfs. We note also the modest value [Ba/Fe] = -0.5 found by Bessell and Norris (1984) for the extraordinary metal-poor star CD $-38^{\circ}245$, for which [Fe/H] = -4.5.

It would be very exciting if it were possible to extract information on the isotopic abundances of barium in extreme metal-poor stars. Prospects using the profile itself are grim. The profiles of the solar and *r*-process mix could be distinguished in a 20 mÅ line with a spectroscopic resolution of the order of 0.03 Å, but only if other sources of broadening were nonexistent. A 1 km s⁻¹ microturbulence (or rotational velocity) virtually washes out the distinction between the profiles with different isotopic mix.

It would be possible in principle to get information on the isotopic mixes if abundances could be very accurately determined from subordinate Ba II as well as the resonance lines. In those stars where the equivalent widths of the resonance lines are most sensitive to the hfs, differences in the abundances determined from the ensemble of Ba II lines could be revealing. The pure *r*-process and solar mixes can differ in log (W) by an amount only the order of 0.1 dex. A credible calculation would be subject to the uncertainties already mentioned. The challenge to the abundance worker is considerable.

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