A RE-EVALUATION OF THE ABUNDANCE OF LUTETIUM IN THE SUN

D. J. BORD[1,*], C. R. COWLEY[2] and D. MIRIJANIAN[1]
[1]*Department of Natural Sciences, University of Michigan-Dearborn, Dearborn, MI 48128, U.S.A.*
[2]*Department of Astronomy, University of Michigan, Ann Arbor, MI 48109, U.S.A.*

(Received 12 June 1997; accepted 22 July 1997)

Abstract. Lutetium is one of the few nonvolatile elements whose solar photospheric abundance departs significantly from that derived from CI chondrites. We have applied the Cowan code to compute new oscillator strengths for Lu II, and have included a correction for core polarization. The results have been used in a synthesis of the solar spectrum in the vicinity of features at $\lambda_\odot$ 3397.062 and $\lambda_\odot$ 6221.72. We find that the majority of the absorption in the ultraviolet feature is due to NH, making it unsuitable for extracting a reliable lutetium abundance. Our best fit to the low-noise Jungfraujoch spectrum for the weak, nine-component hyperfine Lu II line at λ6221.87 yields an abundance of $+0.06$ on a scale where $\log(H) = 12.00$. This value is within 0.07 dex of the meteoritic result ($+0.13$). (These figures reflect the note added in proof below.)

1. Introduction

Abundances of the nonvolatile chemical elements are in close agreement in CI chondrites and the solar photosphere (Grevesse, Noels, and Sauval, 1996, henceforth GNS). The heavy lanthanide lutetium is among the few elements with differences larger than 0.3 dex. GNS give $\log(\mathrm{Lu}_\odot) - \log(\mathrm{Lu}_{\mathrm{CI}}) = 0.63$.

Among the chondrites, the lutetium abundance closely follows that of other refractory elements such as calcium, aluminum, strontium, barium, and the lighter lanthanides (Wasson and Kallemeyn, 1988). A few meteoritic fragments show substantial differences in lanthanide abundances relative to the bulk CI compositions (cf., Palme and Boynton, 1993), but there is little reason to suspect that such differences might be manifested in the photosphere.

Moore, Minnaert, and Houtgast (1966, henceforth MMH) list three Lu II lines: $\lambda_\odot$ 3077.558, $\lambda_\odot$ 3397.062, and $\lambda_\odot$ 3472.457. The first and third features are blends, and the discordant solar abundance rests on the single feature at $\lambda_\odot = 3397.062$. MMH attributed this feature entirely to Lu II, and listed an equivalent width of 28 mÅ. However, Grevesse (1983) suggested that '...Lu II is only a small contributor to the observed solar feature.'

The solar feature at $\lambda_\odot$ 3397.062 falls in the red wing of a stronger Fe I line. The blend is sufficiently close that a separate minimum is not seen. Nevertheless, the feature is distinct enough that one could analyze it by synthesis or even by computing an equivalent width. We measured 27 mÅ by assuming a violet wing symmetrical with the red. This value is very close to that listed by MMH, but nearly

*Department of Astronomy, University of Michigan, Ann Arbor MI, 48109, U.S.A.

Solar Physics **178:** 221–237, 1998.

a factor of two larger than that of Grevesse and Blanquet (1969). Those authors may have used a minimum value for W_λ, knowing that the resulting abundance was already too high.

In the present study, we show that the majority of the absorption at $\lambda_\odot$3397.062 is due to NH, so this ultraviolet feature is not suitable for an abundance determination. However, the very weak Lu II line at λ6221.87 is measurable on low-noise Jungfraujoch spectra, and we have extracted a lutetium abundance from it which reconciles the photospheric abundance with that of the CI chondrites to within $\sim$0.2 dex.

The photospheric Lu abundance is itself still uncertain by about two tenths of a dex, at least half of which is likely due to uncertainties in the oscillator strength of the λ6221 line. We will also discuss the theoretical calculations of the oscillator strengths in Lu II made specifically for the present study. These follow the technique used previously by the authors (cf., Bord, Cowley, and Norquist, 1997), but now include a correction for the effects of core polarization.

2. Atomic Structure Computations

2.1. General methodology

We have continued to employ the general methodology (based on the Cowan (1981, 1995) code) used in our previous studies of La II (Bord, Barisciano, and Cowley, 1996), Ce III (Bord, Cowley, and Norquist, 1997), and Nd III (Cowley and Bord, 1997). Single-particle radial wavefunctions were determined using a Hartree-plus-statistical-exchange-interaction approximation for the following even and odd parity configurations, respectively: $(6s^2 + 5d6s + 5d^2 + 6s7s)$ and $(5d6p + 6s6p)$. These groups include *all* the reliably established configurations for this ion (cf., Martin, Zalubas, and Hagen, 1978). As in the past, relativistic and electron correlation corrections have been included in the calculations, and the eigenvectors were constructed using LS- and jj-coupling basis sets, although the former appears entirely adequate for the description of the known energy levels.

Ab initio values for the single-configuration center-of-gravity energies and the various radial and configuration interaction integrals were optimized by fitting the calculated energy levels to those experimentally known (Martin, Zalubas, and Hagen, 1978) using the method of least squares. We computed 32 levels, of which 30 were fitted; two even levels ($5d^2\ ^1S_0$ and $5d^2\ ^1G_4$) have no well-established experimental values. The adopted structure parameters yielded an average deviation in the fitted energies of 22 cm^{-1} (less than 0.1%) for the 14 even levels, and 32 cm^{-1} (again less than 0.1%) for the 16 odd levels. These parameter values were used to recalculate the energy levels and eigenvectors, which were finally used for improved computations of the wavelengths, transition probabilities, and oscillator strengths.

Our leading eigenvector percentages in LS-coupling are in excellent agreement with those of Goldschmidt (1968) for the $(5d + 6s)^2$ and $(5d6p + 6s6p)$ con-

figurations: the mean difference over the entire set of 28 levels is less than 1%. We confirm that the designations $^3P_2$ and $^1D_2$ in the $5d^2$ configuration have little meaning due to the strong mixing of these terms in the eigenvectors for the levels at 36 098 and 38 575 cm^{-1}. We also substantiate the significant interaction between the $6s6p$ and $5d6p$ configurations reflected in the strong mixture of the $^1P^\circ$ levels in the eigenvectors for the 38 223 and 59 122 cm^{-1} levels, respectively.

Our calculations predict the following energies for the $5d^2\ ^1G_4$ and $5d^2\ ^1S_0$ levels, respectively: 37 616 cm^{-1} and 46 591 cm^{-1}. The former state has a leading eigenvector percentage of 97%, but lies almost 1300 cm^{-1} below the position predicted by Goldschmidt. By contrast, our prediction for the $^1G_4$ level is only 211 cm^{-1} lower than the 37 827 cm^{-1} value suggested by Anderson (1956), which was discarded by Martin, Zalubas, and Hagen (1978) as lacking in convincing experimental evidence. Adopting Anderson's value in our least-squares fitting routine produces an average deviation of 33 cm^{-1} for the 15 even levels fitted, slightly poorer than our previous best fit without this level. Perhaps not unexpectedly, the greatest perturbations are to neighboring $5d^2\ ^3P$ and ^1D levels. We suggest that while Anderson's value may be questionable, it is likely that the correct energy for the $5d^2\ ^1G_4$ level lies closer to 37 616 cm^{-1} than to the $\sim$39 000 cm^{-1} figure given by Mrs Goldschmidt.

2.2. CORE POLARIZATION CORRECTIONS AND RADIATIVE LIFETIMES

Previous papers have discussed the limitations on the accuracy of our radiative lifetimes and oscillator strengths due to inadequate compensation for core polarization. Specifically, the calculated lifetimes tend to be too short, often by up to a factor of 2 or slightly more, when compared with experimental values. In an attempt to correct for core polarization effects in Lu II, we have determined correction factors for our radiative lifetimes and gf-values from comparisons between our transition array values and those derived using a multi-configuration Hartree-Fock (MCHF) approach with model potentials to describe the core polarization contributions (Vaeck, Godefroid, and Froese Fischer, 1992). The form of the model potentials follows that introduced by Hameed (1972) and Baylis (1977), and requires the specification of two parameters: the dipole polarizability of the core, α, and a cut-off radius, r_c, for the correction terms in the potential for the valence electrons. As is common in applications of this type, for the first parameter we have used the value for the static dipole polarizability computed by Johnson (1997), viz., $4.265a_0^3$, where a_0 is the radius of the first Bohr orbit of hydrogen.

Brage and Froese Fischer (1992) have pointed out that there is no specific, *a priori* method for selecting the cut-off radius. In *ab initio* computations, the cut-off radius is often taken to be the expectation value of r for the outer-most core orbitals (cf., Hibbert, 1989); sometimes semi-empirical calculations are performed wherein the cut-off is adjusted to reproduce known values for the transition energies, ionization energies, etc. (cf., Vaeck, Godefroid, and Froese Fischer, 1992). For this

Table I
Radiative lifetimes for selected $5d6p$ states of Lu II

State	Energy (cm^{-1})	λ (Å)	τ (ns)	τ_{exp} [a] (ns)
$^3F_2^\circ$	41225	3397	5.18	3.7 ± 0.4
$^3F_3^\circ$	44919	3077, 3254	4.21	3.8 ± 0.5
$^1D_2^\circ$	45459	3554	3.92	2.8 ± 0.3
$^3D_1^\circ$	45532	3020	2.51	2.4 ± 0.3
$^3D_2^\circ$	46904	2847, 3057	3.01	3.8 ± 0.5
$^3F_4^\circ$	48537	2911	3.25	4.2 ± 0.4
$^3D_3^\circ$	48733	2754, 2894	2.91	4.0 ± 0.5
$^3P_1^\circ$	50049	2613, 2657	1.94	3.4 ± 0.5

Based on beam-foil measurements reported by Andersen and Sørensen (1974) and Andersen *et al.* (1975).

analysis, we have adopted a value of $1.409a_0$ for the cut-off; this equals the average value of $\langle r \rangle$ for the outer-most core orbitals ($5p^6$) for the six valence configurations investigated as determined by the program RCN2 in the Cowan (1995) code. Although not optimized to reproduce any specific experimental parameter values for Lu II, this choice provides reasonable agreement with measured lifetimes for $5d6p$ levels (see below), and, in the light of the investigations of Brage and Froese Fischer (1992), is not likely to reduce the oscillator strengths to unacceptably low values. Tests of the sensitivity of our correction factors to a 10% variation in the value of the cut-off radius revealed no changes greater than ∼5%.

Our choices for α and r_c differ from those adopted by Migdalek and Baylis (1988) in their multi-configuration Dirac–Fock calculations of $6s^2\,{}^1S_0 - 6s6p\,{}^3P_1^\circ$, ${}^1P_1^\circ$ transitions in Lu II. They took $\alpha = 5.20a_0^3$ from Fraga, Karwowski, and Saxena (1976) and $r_c = 1.413a_0$, the mean radius of the unpolarized Lu^{3+} ion. We compare our oscillator strengths to theirs in the next subsection.

As expected, the core polarization corrections reduced the transition array values produced by the Cowan code, and yielded a scaling factor for the radiative lifetimes of upper levels in $5d6s - 5d6p$ transitions of 1.13. Similar sized scaling factors were found for $6s^2 - 6s6p$ and $5d6s - 6s6p$ transitions. The corrected lifetimes for selected $5d6p$ states are displayed in Table I. The final column of the table shows the lifetime measurements for this ion reported by Andersen and Sørensen (1974) and Andersen, Poulsen, Ramanujam, and Petrakiev Petkov (1975) based on beam-foil experiments.

Figure 1 compares the calculated lifetimes from Table I to the beam-foil measurements in terms of the ratio, R, of the experimental values to the computed ones, as a function of level energy. The error bars reflect the reported uncertainty in the beam-foil results plus an *assumed* 15% uncertainty in our calculations. With the exceptions of the $^3F_2^\circ$ level at 41 225 cm^{-1}, the $^1D_2^\circ$ level at 45 459 cm^{-1},

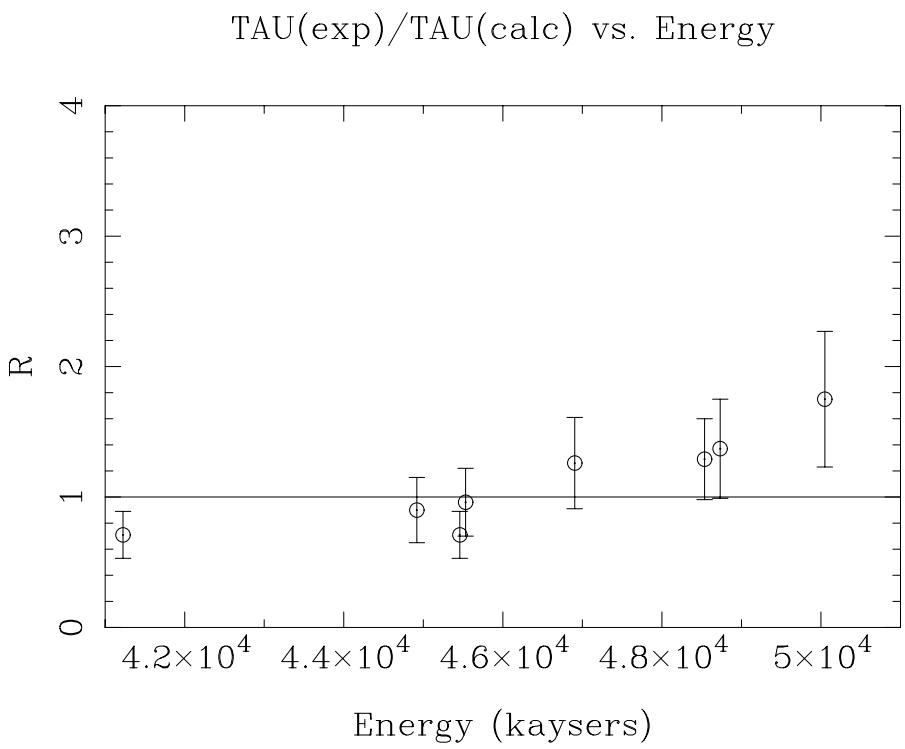

Figure 1. The ratio R of the measured to the calculated lifetime as a function of energy for eight levels in the 5*d*6*p* configuration of Lu II. Error bars reflect the reported experimental uncertainties in the beam-foil measurements plus an assumed 15% uncertainty in the computed lifetimes.

and the $^3P_1^\circ$ level at 50 049 cm^{-1}, a value of $R = 1.00$ can be accommodated within the uncertainties of the remaining data points. Even including all the points, the mean value of R is 1.12 ± 0.36, consistent with a unit ratio to within 30%, typical of the uncertainty in the individual values of R. If the $^3P_1^\circ$ lifetime is discarded, the remaining seven points yield $R = 1.03 \pm 0.28$. These results compare very favorably to those of Pinnington, Livingston, and Kernahan (1974) who found $R = 1.11 \pm 0.18$ for 46 different mean beam-foil lifetimes for five different elements.

The failure to reconcile the values of R for the $^3F_2^\circ$ and $^1D_2^\circ$ levels with unity is likely due to larger than estimated uncertainties in the calculated lifetimes having to do with the low purity of these states: the eigenvector for each state contains an approximately 25% admixture of the other. The beam-foil lifetime for the $^1D_2^\circ$ level appears quite reliable in the light of the Hanle-effect lifetime of 2.8 ± 0.4 ns for this state found by Andersen *et al.* (1975). The disagreement exhibited by the $^3P_1^\circ$ level may reflect incomplete correction for experimental uncertainties. Upper levels like this one require higher beam energies to excite and therefore are more susceptible to errors arising from insufficient correction for energy losses in the

foil and to greater uncertainties produced by more complex cascade corrections (Sørensen, 1976). The computed $^3P_1^\circ$ lifetime should not contain any pronounced uncertainties beyond those already included in our estimate insofar as this state is essentially pure; tests of the stability of the computed lifetime to the inclusion of possible higher energy configurations (see Bovey and Pearce, 1956) reveal no changes at the level of a percent or less.

Figure 1 also reveals what appears to be a trend toward increasing values of R with increasing level energy over the $\sim$9000 cm^{-1} range covered by the data. We have not observed such behavior before in the distribution of lifetime ratios with energy (cf., Bord, Barisciano, and Cowley, 1996; Bord, Cowley, and Norquist, 1997), and we do not attach too much significance to it in the light of the uncertainties in the data and the limited range of energy involved. A portion of the putative trend is certainly due to our use of a mean correction to the $5d6s - 5d6p$ transition array in lieu of separate corrections for the reduced matrix elements of the various multiplets within this array. This tends to overcorrect some levels and undercorrect others relative to the mean, but only within very narrow limits. The individual correction factors deviate from the mean one for the array by only $\leq$5%.

2.3. OSCILLATOR STRENGTHS

Our core polarization corrections increase the computed lifetime data and concomitantly decrease the oscillator strengths. For example, a 13% rise in the lifetimes of the $5d6p$ states corresponds to a 0.053 reduction in the $\log(gf)$ values for transitions involving these levels. Table II presents the corrected oscillator strengths for the strongest lines in the second spectrum of lutetium.

Mindful of the problems that can beset theoretical oscillator strengths for certain kinds of transitions in complex ions, we have reported in Table II $\log(gf)$ values for lines which do not involve intersystem transitions and for which the cancellation factors (cf., Cowan, 1981; Equation (14.107)) are all greater than 0.4. We have also restricted our list to lines having intensities of at least 1000 on the system adopted by Reader and Corliss (1980); these features are likely to be of greatest astrophysical interest. A complete list of gf-values for all allowed transitions arising from the configurations included in our analysis is available from the authors upon request.

As far as we are aware, aside from the work of Corliss and Bozman (1962, hereafter CB), there are no experimental oscillator strengths available with which to compare our results. For the data provided in Table II, we find that our $\log(gf)$ values are 0.27 dex smaller on average than those given by CB for wavelengths below 3600 Å; for the three lines with $\lambda >$5400 Å, our $\log(gf)$'s are all larger than the CB values by $\sim$0.5 dex. Andersen and Sørensen (1974) and Andersen *et al.* (1975) have calculated lifetimes for the $5d6p$ transitions included in Table I using the CB data. Excepting the $^3F_2^\circ$ level at 41 225 cm^{-1} for which the ratio $R \equiv \tau_{\text{beam-foil}}/\tau_{\text{CB}} = 0.82 \pm 0.09$, the remaining seven states all have beam-foil

Table II
gf-values for prominent lines in the second spectrum of lutetium

λ_{air} (Å)	Intensity[a]	Transition	$\log(gf)$
2392.19	1300	$17333_2 - 59122_1^\circ$	0.176
2578.79	1700	$12435_2 - 51202_2^\circ$	−0.227
2613.40	1800	$11796_1 - 50049_1^\circ$	−0.186
2615.42	18000	$0_0 - 38223_1^\circ$	0.195
2619.26	1800	$11796_1 - 49964_0^\circ$	−0.301
2657.80	2700	$12435_2 - 50049_1^\circ$	−0.094
2701.71	4200	$14199_3 - 51202_2^\circ$	0.141
2754.17	3600	$12435_2 - 48733_3^\circ$	0.002
2796.63	2700	$17333_2 - 53079_3^\circ$	0.238
2847.51	3000	$11796_1 - 46904_2^\circ$	−0.239
2894.84	6300	$14199_3 - 48733_3^\circ$	0.175
2900.30	4500	$12435_2 - 46904_2^\circ$	−0.126
2911.39	9000	$14199_3 - 48537_4^\circ$	0.527
2963.32	4200	$11796_1 - 45532_1^\circ$	−0.235
3020.54	3000	$12435_2 - 45532_1^\circ$	−0.325
3056.72	2100	$14199_3 - 46904_2^\circ$	−0.240
3077.60	7500	$12435_2 - 44919_3^\circ$	0.183
3254.31	4800	$14199_3 - 44919_3^\circ$	−0.161
3397.07	4100	$11796_1 - 41225_2^\circ$	−0.098
3472.48	4800	$12435_2 - 41225_2^\circ$	−0.214
3554.43	4800	$17333_2 - 45459_2^\circ$	−0.269
5476.69	2100	$14199_3 - 32453_2^\circ$	−0.276
6221.87	2100	$12435_2 - 28503_1^\circ$	−0.604
6463.12	1100	$11796_1 - 27264_0^\circ$	−0.926

[a] As reported by Reader and Corliss (1980). Only lines with intensity $\geq$1000 are included here.

lifetimes that exceed the CB values by factors of from 1.90 up to 3.78. This is in sharp contrast to the results presented in Figure 1.

A least-squares fit of the data in Table II of the form

$$\log(gf) - \log(I\lambda^3) = a + bE_{\text{upper}}$$

yields $a = -17.20$, and $b = (6.73 \pm 0.44) \times 10^{-5}$. The standard error of the fit is 0.16 dex, comparable to the uncertainties reported in similar intensity calibration studies (cf., Cowley and Corliss, 1983; Bord, Barisciano, and Cowley, 1996). The temperature that is implied by the b-coefficient is 9282 K, higher than any found by Cowley and Corliss. Consequently, some caution must thus be exercised in using the above equation to produce oscillator strengths for lines not included in Table II.

On the basis of our past experience with fits of this kind, and also the discussion below, we recommend using $a = -17.35$.

Migdalek and Baylis (1988) report the following oscillator strengths for the $6s^2\,{}^1S_0$ to $6s6p\,{}^1P_1^\circ$ and ${}^3P_1^\circ$ transitions, respectively, using experimental excitation energies: 1.30 and 0.0657. The corresponding $\log(gf)$ values are $+0.114$ and -1.182. Table II gives $\log(gf) = +0.195$ for the ${}^1S_0 - {}^1P_1^\circ$ transition; the semi-forbidden ${}^1S_0 - {}^3P_1^\circ$ line is not included in Table II, but our calculations yield a value of -1.093 for the $\log(gf)$.

A part of the difference between our results and those of Migdalek and Baylis is due to our use of a smaller dipole polarizability. We have recomputed our core polarization correction for these transitions using $\alpha = 5.20a_0^3$ and find $\log(gf) = +0.183$ for the ${}^1S_0 - {}^1P_1^\circ$ transition and $\log(gf) = -1.105$ for the ${}^1S_0 - {}^3P_1^\circ$ one. Based on these numbers, our calculations are $\sim$18% larger than those of Migdalek and Baylis. In the light of the acknowledged configuration interaction present in the $6s6p\,{}^1P_1^\circ$ state and the intersystem character of the ${}^1S_0 - {}^3P_1^\circ$ transition, we consider this agreement quite satisfactory.

Based on the results of the comparisons between the computed and measured lifetimes for this ion and between our computed gf-values and the theoretical ones produced by Migdalek and Baylis, we expect that the tabulated oscillator strengths should be good to $\leq$25% or about 0.1 dex, but that they may still be systematically too large on average.

3. Calculation of the Synthetic Solar Spectrum

The programs used for the present study are essentially the same as those described by Cowley (1996), based on LTE. For the Sun, we made appropriate modifications to the flux codes to get the spectrum in the specific intensity. All calculations were made in double precision. Our model atmosphere was constructed from the temperature distribution given by Holweger and Müller (1974), which has been widely used for photospheric abundances by Grevesse and his co-workers as well as others (cf., Gratton and Sneden, 1994).

Only diatomic H_2 is included in the pressure-depth calculation. For the synthesis, equilibria for 10 diatomic radicals of H, C, N, and O, plus H_2O, CO_2, CH_2, C_2H, and C_2H_2 were calculated at each depth using the constants of Tsuji (1973, 1997). We used the partition function interpolation coefficients of Sauval and Tatum (1984) for NH, the only molecule of importance in the present work. These parameters fit identified NH lines in the region (e.g., $\lambda\lambda$3395.27, 3395.75) with no adjustments. Since, in the present study, we have not attempted an abundance for nitrogen, we have not looked into updates of the molecular parameters.

A good way to test a solar model atmosphere is to compare the computed emergent intensity with measurements reported by Neckel and Labs (1984). At a wavelength of 3397 Å, we obtain a continuum specific intensity of 4.19×10^{14} c.g.s.

(erg cm^{-2} s^{-1} sterad^{-1} cm^{-1}). From Neckel and Labs' Table III, we find for 3398.25 Å the value $\Sigma = 4.18$ in units of watts cm^{-2} sterad^{-1} per 20.5 Å band. To convert to our units we divide by 20.5×10^{-15}. The result is 2.04×10^{14} c.g.s., which includes the effects of line blocking.

We estimate the amount of line blocking by integrating over a 5 Å region of the digitized Jungfraujoch spectrum (cf., Delbouille and Roland, 1995) kindly supplied to us by Grevesse and Sauval (1997). In this region, only a fraction, 0.654, of the entire 'continuum' is emitted. Allen (1976) tabulated 0.64 for this fraction. If we diminish our value by 0.654, we find 2.74×10^{14} c.g.s., too high by 34.3%. This is an example of the well-known 'missing' ultraviolet opacity of the Sun.

It would be possible to compensate for this missing opacity by scaling our calculated continuous opacity until we matched the observations. The result, for a 27 mÅ line, of increasing the continuous opacity at all depths by 40% would be to increase the resulting abundance by 0.04 dex. The missing opacity is not a critical problem for an abundance that is discordant by 0.6 dex. Since we shall find below that the λ3397 region is not suitable for assessing the lutetium abundance, we need not pursue this.

At λ6222, the calculated emergent intensity is 3.16×10^{14} c.g.s. The measured value from Neckel and Labs is 3.03×10^{14} c.g.s. We reduce the theoretical value by 0.966 to account for blocking. This value comes from an integration over 20.46 Å of the theoretical spectrum with standard abundances, but it is essentially the same as that (0.97) listed by Allen (1976) for this region. We find, then, 3.05×10^{14} c.g.s., in good agreement with the measured intensity.

4. Analysis of the $\lambda_\odot$3397 Blend

The solid line in Figure 2 shows the region of the putative Lu II line as observed at the Jungfraujoch. The dashed line represents a synthesis using standard abundances (SAD) from GNS. Atomic and molecular data were taken from the CD-Roms of Kurucz (1993); for lutetium the data provided in Section 2 were used. No molecules were used in the generation of the dashed spectrum. The dotted line in Figure 2 shows calculations of the spectrum excluding Lu II, but it includes five lines of NH from the system $A^3\Pi - X^3\Sigma^-$.

Apart from dropping the Lu II and including NH lines, we modified the transition probability for Fe I λ3397.56. This is an intersystem transition between levels at 24 338.765 and 53 763.276 cm^{-1} ($b^3G_3 - x^1F_3^\circ$), according to Nave *et al.* (1994). The value of $\log(gf)$ for this line given by Kurucz is -4.66, while that used to calculate the dotted spectrum was -2.00, 2.66 dex larger. While an underestimate of the oscillator strength for an intersystem transition of this magnitude is not without precedent, it is also possible that absorbers other than Fe I are at least partly responsible for the feature.

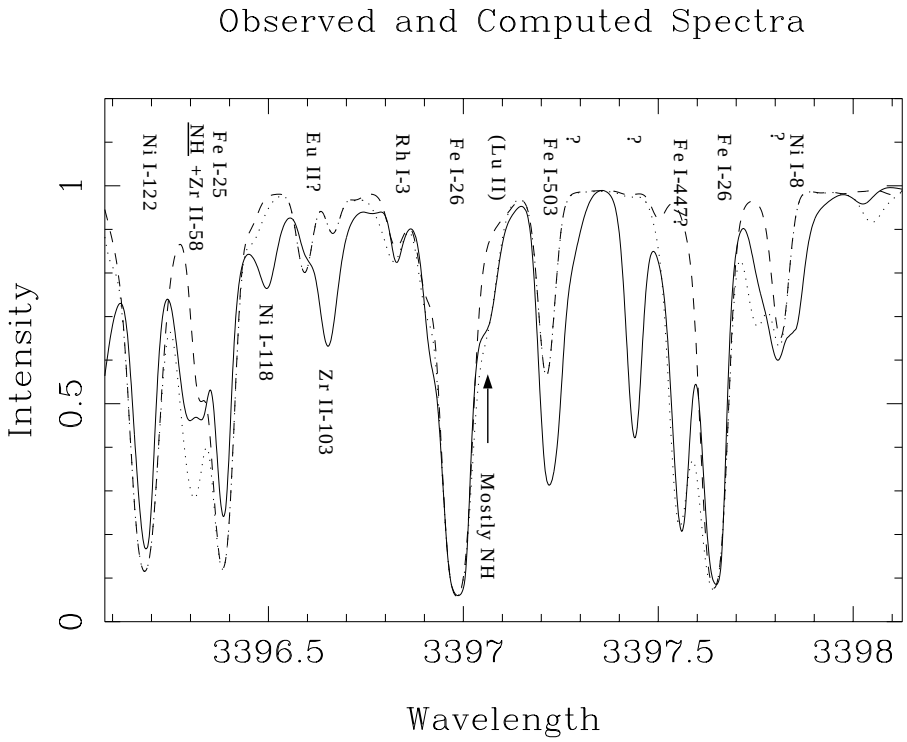

Figure 2. The solid line is the observed solar spectrum near Lu II λ3397. Identifications are from MMH. The dashed spectrum was computed with no NH, while the dotted one includes NH, but not Lu II. The dotted curve also reflects an increased $\log(gf)$ for the intersystem Fe I line at 3397.56 Å from -4.66 to -2.00 (see text). Apart from this change, the calculation is 'raw' in the sense that abundances, atomic and molecular parameters, and computing algorithms have not been adjusted to improve the fits.

It is clear that NH could account for all the absorption at $\lambda_{\odot}$3397.06 once attributed to Lu II. If we make a close comparison of the dotted and dashed portions of Figure 2, we see that the NH absorption slightly overshoots the observations in at least two regions. In Figure 3, we have attempted a best fit to the blend. This involved making adjustments of up to 0.01 Å in the mean position of the Lu II 'line', which is actually a blend of hyperfine components. (See remarks below on the wavelength of a hyperfine-split line.) The structure of the lower level of this line is known (Brix and Kopfermann, 1952). Our calculations assumed the upper level was unsplit. In addition to small adjustments of the Lu II components, we recalculated the oscillator strength of the NH line, and took its position (λ3397.054) from the work of Brazier, Ram, and Bernath (1986). The NH abundance used in Figure 3 is 60% of the equilibrium value for this molecule derived from the solar abundances of H and N.

Remarkably, Kurucz's work, based on older studies of NH, predicted the position of the critical line to within 0.024 Å of the more modern wavelength. Although

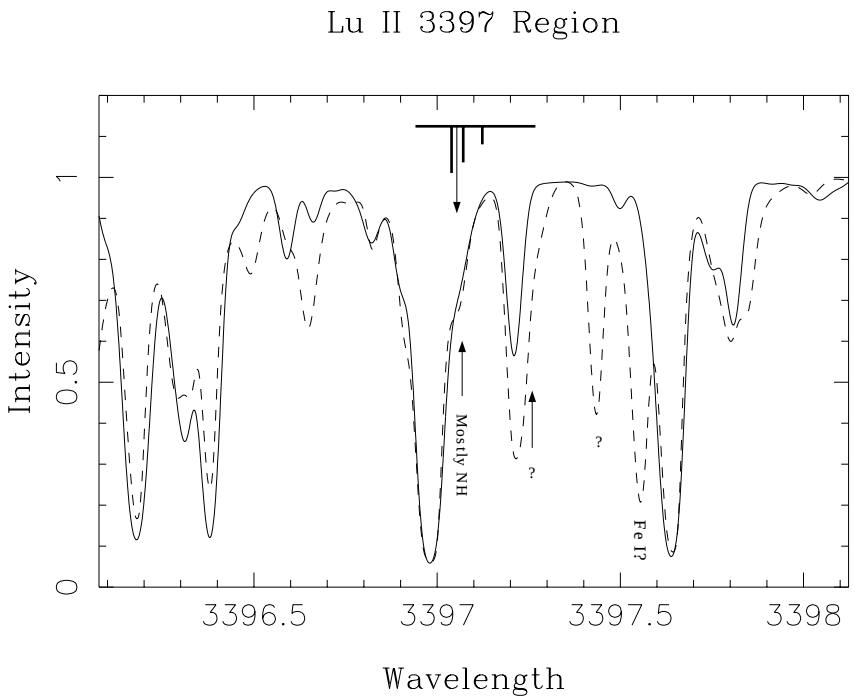

Figure 3. Optimized fit (solid) to the λ3397.06 region. Note that the observed spectrum is now dashed. The best fit was obtained with the NH abundance reduced by a factor of 0.6 from its equilibrium value derived using the solar abundances of N and H. The hyperfine pattern for the Lu II feature is shown under the assumption that the upper level is unsplit. An arrow shows the position of the molecular line. In view of the general unsuitability of this region, no attempt was made to improve the fit or account for possible predissociation broadening of the NH line. Absorptions of unknown or uncertain origin are indicated by question marks.

Figures 2 and 3 use Kurucz's oscillator strengths, we did check the value for the NH λ3397.054-line using $A_{n'n''} = 4.11 \times 10^6$ as tabulated by Lents (1973). We used the rotational strength from the program by Whiting (1973). The result was $\log(gf) = -0.61$; Kurucz had given -0.55. This particular NH line is in the Q_3 branch of the (2–2) band, $J' = 17$ to $J'' = 17$.

The molecular transition could be affected by predissociation, for which we have not allowed. A better fit might well be made, but in view of the overall unsuitability of this region for a lutetium abundance, we have not attempted further adjustments. A surprising amount of absorption in this region remains unexplained, even after adding NH and CH. If other molecules are responsible, they are not in the Kurucz data base.

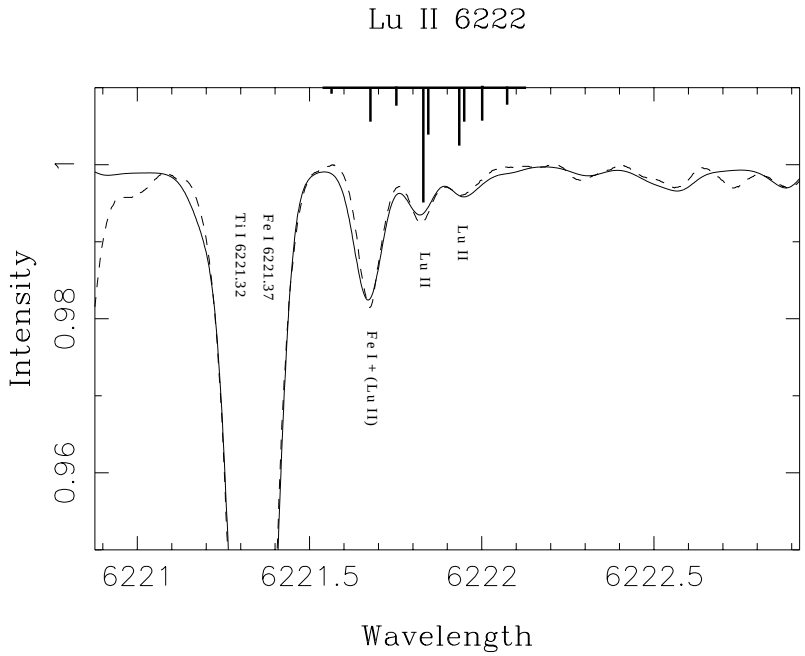

Figure 4. The weak Lu II feature at λ6221.87 is split by the hyperfine structure shown. Only the top 5% of the continuum is shown. The computed spectrum is again the solid line, and the observed spectrum is dashed. Minor adjustments ($\leq$ 0.01 Å) have been made to the the wavelengths of atomic lines, as discussed in the text. The adopted lutetium abundance is -0.10 on a scale of $\log(H) = 12.00$.

5. The Weak Lu II Line λ6221.87

Lu II λ6221.87 was not identified by MMH, but the stronger component of this complex feature was probably what was measured at $\lambda_\odot$6221.72. Hyperfine splitting is known for both the upper and lower levels of this transition ($5d6s\,^3D_2 - 6s6p\,^3P^\circ_1$); all together, there are nine hyperfine components.

Figure 4 shows the top 95% of the solar spectrum, obtained over the 'net' from the French Solar Data Base (BASS, http://mesola.obspm.fr). It is essentially the same Jungfraujoch material that we obtained from Grevesse and Sauval, except that in the previous case, our colleagues had chosen the continuum for us.

BASS makes a digital spectrum available as integers from 0 to 10 000 with spacings of 2 mÅ. For the λ6222 region we adopted a continuum at 9913; this is essentially the maximum value reached over a 5 Å region.

The nine hyperfine components are shown in Figure 4, with intensities drawn approximately to scale. The positions of the components were set as follows. We computed splittings (in cm^{-1}) for the upper and lower levels from the A and B parameters given by Brix and Kopfermann. These were added and subtracted, respectively, from the 'mean position' of the line (also in cm^{-1}). The appropriate mean position for a hyperfine-split line is not obvious. Reader and Corliss (1980)

list 6221.87 Å. By subtracting the energy levels given by Martin, Zalubas, and Hagan (1978), we obtain 6221.891 Å. A best fit to the solar features was obtained with the value 6221.86 Å; this is what is illustrated in Figure 4.

The calculated spectrum includes a line due to Nb I, λ6221.90. It has a hyperfine width of about 0.1 Å (Litzen 1997). The oscillator strength is from Kurucz and Bell (1995). Their value was adjusted from the listing of CB to account for the measured lifetimes in Nb I of Duquette and Lawler (1982). This line is too weak to affect the lutetium abundance determination.

Data of the quality of the Jungfraujoch spectra are a challenge to analyze for several reasons. One can surely measure wavelengths to a milliangstrom (or so), but the atomic lines are often uncertain by 10 or more milliangstroms. The wavelengths are known to depend on the laboratory source, a problem that may be paliated by the use of wavelengths generated from energy levels. There is the additional problem of the registration of the digitized theoretical and observed tracings, which we usually do by a cross correlation of the theoretical and observed spectra. In this endeavor, one hopes the errors of the atomic lines will cancel. In the present work, we used only small regions of the spectrum, and did not attempt to reset the wavelength zero points of Grevesse and Sauval or Meudon.

The lutetium abundance leading to the fit of Figure 4 is -0.10 on the usual scale where $\log(H) = 12.0$. This value is obtained with the theoretical calculation of $\log(gf) = -0.604$ for the line, taken from Table II. (For comparison, CB give $\log(gf) = -1.11$ for the λ6222 line; this is also the value reported in Kurucz and Peytremann (1975) and in the file BELLHEAVY.DAT (Kurucz and Bell, 1995).) GNS give $+0.13 \pm 0.02$ for the meteoritic abundance, so the discrepancy is now only a little over 0.2 dex. At least half of this difference is likely due to uncertainties in the oscillator strength of the λ6221.87 line; the remainder very well lies with cumulative uncertainties in the choices of the parameters used in the model atmosphere and synthesis calculations and the fitting of the theoretical and observed spectrum.

6. Conclusions

Figure 5 illustrates the relation between the photospheric and CI meteoritic abundances of lutetium prior to and after the present work. We have already mentioned a suggestion that the λ3397 line was blended, but until the blend was identified, we could not be certain of the nature of the discrepancy. We are unaware of an earlier use of the λ6222 line for abundance purposes.

In Figure 5 we plot the logarithmic solar abundances from GNS minus CI abundances from the compilation of McDonough and Sun (1995). The latter group has not been involved with the reconcilation of solar and meteoritic abundances, but their values are very close to those of Anders and Grevesse (1989). The differences are plotted versus elemental condensation temperatures. These are mostly from

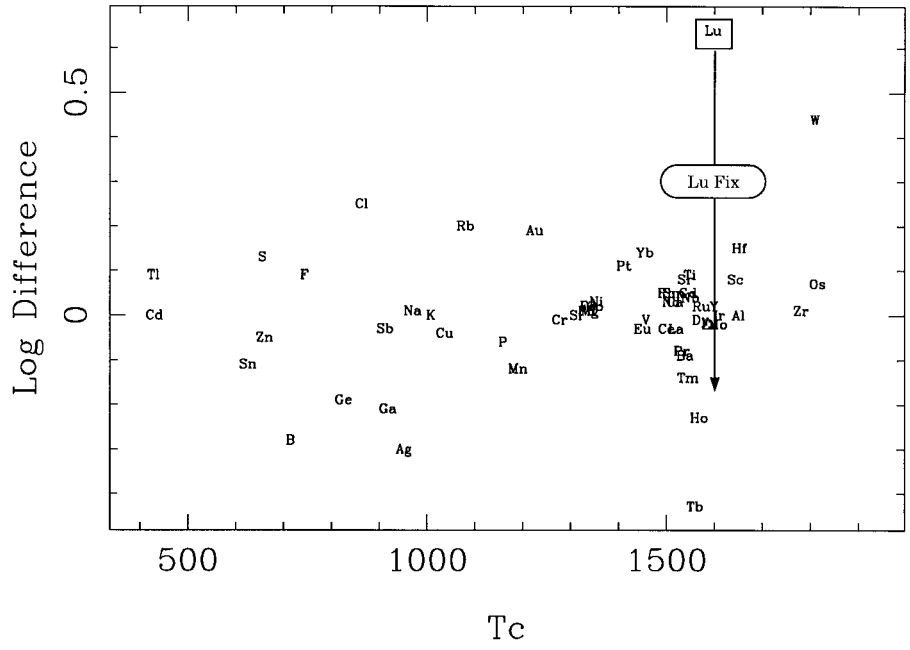

Figure 5. Logarithmic photospheric (GNS) minus CI abundances (from McDonough and Sun, 1995) vs elemental condensation temperatures, mostly from Wasson (1985). Points are indicated by chemical symbols of the elements. The position of lutetium prior to and after the present work is shown by the arrow.

Wasson (1985), but values for Sr, Rh, In, I, Cs, Ba, Ta, Tl, and Bi are estimates. The estimates were based on the correlation of the abundances of these elements with others of known condensation temperatures in averages for 9 chondrites given by Wasson and Kallemeyn (1988). For example, indium correlates well with Br, Zn, Ag, Ce, Sn, and Te and the estimate of $T_c = 673$ K is the average of the T_c's for these elements. Barium and strontium correlate well with the rare earths, so we assume $T_c = 1539$ K, a mean for these elements.

A modern experimental determination of the transition probability for λ6222 may bring the photospheric abundance into even closer agreement with the CI's than our current best estimate. Such measurements are being undertaken as these lines are written (Lawler 1997). At the level of a tenth of a dex, various additional factors become relevant that have previously been unimportant. These are the solar model itself, the assumption of LTE, unmeasured hyperfine structure, details of the fitting procedure involving instrumental broadening, micro- and macroturbulence, etc.

It is puzzling why the abundances of the CI meteorites mimic the photospheric composition so faithfully. The meteorites are well known to have a complex chemical history in which aqueous alteration has played the dominant role. Somehow, the bulk compositions of these samples are largely unfractionated. As our know-

ledge of the solar abundances increases, we should gain insight into the history of these remarkable objects.

Acknowledgements

The authors are deeply indebted to the following individuals for their advice and assistance during the course of this project: Dr Tomas Brage for providing the programs with which the core polarization corrections were done and for instructing us in their proper use; Dr Walter Johnson for computing the dipole polarizability for the core configuration of Lu II at our request; Dr William Martin for providing copies of several of the more obscure references for lutetium and for helpful commentary regarding the analysis of the spectrum of this element; Drs N. Grevesse and A. Sauval for providing the Jungfraujoch spectrum of the Sun in the vicinity of the $\lambda_{\odot}$3397.052 feature and for their comments on a draft of this manuscript; Dr Peter Bernath and Jens Hohmann for help with the NH molecule; and Dr Robert Kurucz for his CD-ROMS. To each of them we extend our sincere thanks and appreciation.

Note Added in Proof

As this paper was being refereed for publication, we were privileged to receive the results of experimental lifetime and branching ratio measurements in Lu II made by Dr J. E. Lawler and his collaborators at the University of Wisconsin. Of particular relevance to our study is the lifetime of the $6s6p\,^3P_1^{\circ}$ level at 28 503.16 cm^{-1} and the transition probability for the λ6222 line out of this level. Den Hartog *et al.* (1998) give $\tau_{28503} = 37.4 \pm 1.9$ ns based on decay curves for the λ6222 and λ3507 lines, and $\log(gf) = -0.76 \pm 0.04$ for λ6222 using weighted mean branching ratios obtained from FTS data acquired at the National Solar Observatory.

We calculate a core-polarization-corrected lifetime of 28.8 ns for the 28503 cm^{-1} state, yielding a ratio R of experiment to theory of 1.29. This is comparable to the values of R reported earlier in this paper.

The experimental $\log(gf)$ for the critical λ6222 line in Lu II is 0.16 dex smaller than the value we computed and used to establish the solar lutetium abundance. Adopting the new value raises the abundance by precisely this difference to $+0.06$ dex to two significant digits. Although residual uncertainties of ± 0.10 dex still probably exist, this result is within 0.07 dex of the meteoritic value given by GNS.

It is a great pleasure to thank Dr James E. Lawler and Dr Elizabeth A. Den Hartog for their interest in this problem and for their willingness to make the results of their experiments available to us in advance of publication.

References

Allen, C. W.: 1976, *Astrophysical Quantities*, 3rd ed., Athlone Press, London, p. 172.
Anders, E. and Grevesse, N.: 1989, *Geochim. Cosmochim. Acta* **53**, 197.
Anderson, J.: 1956, Thesis, Imperial College, London, 89 pp.
Andersen, T. and Sørensen, G.: 1974, *Solar Phys.* **38**, 343.
Andersen, T., Poulsen, O., Ramanujam, P. S., and Petrakiev Petkov, A.: 1975, *Solar Phys.* **44**, 257.
Baylis, W. E.: 1977, *J. Phys. B: At. Mol. Phys.* **10**, L583.
Bord, D. J., Barisciano, L. P., Jr., and Cowley, C. R.: 1996, *Monthly Notices Roy. Astron. Soc.* **278**, 997.
Bord, D. J., Cowley, C. R., and Norquist, P. L.: 1997, *Monthly Notices Roy. Astron. Soc.* **284**, 869.
Bovey, L. F. H. and Pearse, R. W. B.: 1956, U.K. Atomic Energy Research Establishment Rep. AERE C/R 1976, Harwell, 19 pp.
Brage, T. and Froese Fischer, C.: 1992, *Phys. Scripta* **45**, 43.
Brazier, C. R., Ram, R. S., and Bernath, P. F.: 1986, *J. Mol. Spectr.* **120**, 381.
Brix, P. and Kopfermann, H.: 1952, in Landolt-Börnstein, *Zahlenwerte und Funktionen*, 6th ed., Vol. I, Part 5, Springer-Verlag, Berlin.
Corliss, C. H. and Bozman, W. R.: 1962, *Experimental Transition Probabilities for Spectral Lines of Seventy Elements*, N.B.S. Monograph **53**, U.S. Gov. Print. Off., Washington (CB).
Cowan, R. D.: 1981, *The Theory of Atomic Structure and Spectra*, University California Press, Berkeley.
Cowan, R. D.: 1995, Programs RCN/RCN2/RCG/RCE, Los Alamos National Laboratory (May 1995).
Cowley, C. R.: 1996, in S. J. Adelman, F. Kupka, and W. W. Weiss (eds), *Model Atmospheres and Spectrum Synthesis: 5th Vienna Workshop*, Astron. Soc. Pacific, San Francisco, p. 170.
Cowley, C. R. and Bord, D. J.: 1997, in J. C. Brandt, T. B. Ake, and C. C. Petersen (eds), *The Scientific Impact of the Goddard High Resolution Spectrograph*, ASP Conf. Series, in press.
Cowley, C. R. and Corliss, C. H.: 1983, *Monthly Notices Roy. Astron. Soc.* **203**, 651.
Delbouille, L. and Roland, G.: 1995, in A. J. Sauval, R. Blomme, and N. Grevesse (eds), *Laboratory and Astronomical High Resolution Spectra*, ASP Conf. Series, Vol. 81, p. 32.
Den Hartog, E. A., Curry, J. J., Wickliffe, M. E., and Lawler, J. E.: 1998, *Solar Phys.* **178**, 239 (this issue).
Duquette, D. W. and Lawler, J. E.: 1982, *Phys. Rev. A* **26**, 330.
Fraga, S., Karwowski, J., and Saxena, K. M. S.: 1976, *Handbook of Atomic Data*, Elsevier, Amsterdam, Table VI(1), p. 323.
Goldschmidt, Z. B.: 1968, Thesis, Hebrew University, Jerusalem, 487 pp.
Gratton, R. G. and Sneden, C.: 1994, *Astron. Astrophys.* **287**, 927.
Grevesse, N.: 1983, *Phys. Scripta* **T8**, 49.
Grevesse, N. and Blanquet, G.: 1969, *Solar Phys.* **8**, 5.
Grevesse, N. and Sauval, A. J.: 1997, private communication.
Grevesse, N., Noels, A., and Sauval, A. J.: 1996, in S. Holt and G. Sonnenborn (eds), *Cosmic Abundances*, ASP Conf. Series, Vol. 99, p. 117 (GNS).
Hameed, S.: 1972, *J. Phys. B: At. Mol. Phys.* **5**, 746.
Hibbert, A.: 1989, *Phys. Scripta* **39**, 574.
Holweger, H. and Müller, E. A.: 1974, *Solar Phys.* **39**, 19.
Johnson, W. R.: 1997, private communication.
Kurucz, R. L.: 1993, CD-ROM Nos. 15 and 18, Smithsonian Astrophys. Obs., Cambridge, MA.
Kurucz, R. L. and Bell, B.: 1995, CD-ROM No. 23, Smithsonian Astrophys. Obs., Cambridge, MA.
Kurucz, R. L. and Peytremann, E.: 1975, *Smithsonian Astrophys. Obs. Spec. Rept.* **362**.
Lawler, J. E.: 1997, private communication.
Lents, J. M.: 1973, *J. Quant. Spectr. Radiat. Transfer* **13**, 297.
Litzen, U.: 1997, private communication.
Martin, W. C., Zalubas, R., and Hagan, L.: 1978, *Atomic Energy Levels–The Rare Earth Elements*, NSRDS-NBS **60**, U.S. Gov. Print. Off., Washington.
McDonough, W. F. and Sun, S.-S.: 1995, *Chem. Geol.* **120**, 223.
Migdalek, J. and Baylis, W. E.: 1988, *J. Quant. Spectr. Radiat. Transfer* **37**, 521.

Moore, C. E., Minnaert, M. G. J., and Houtgast, J.: 1966, *The Solar Spectrum 2935 Å to 8770 Å*, N.B.S. Monograph **61**, U.S. Gov. Print. Off., Washington (MMH).
Nave, G., Johansson, S., Learner, R. C. M., and Brault, J. W.: 1994, *Astrophys. J. Suppl.* **94**, 221.
Neckel, H. and Labs, D.: 1984, *Solar Phys.* **90**, 205.
Palme, H. and Boynton, W. V.: 1993, in E. H. Levy and J. I. Lunine (eds), *Protostars and Planets III*, University Arizona Press, Tucson AZ, p. 979.
Pinnington, E. H., Livingston, A. E., and Kernahan, J. A.: 1974, *Phys. Rev. A* **9**, 1004.
Reader, J. and Corliss, C. H.: 1980, *Wavelengths and Transition Probabilities for Atoms and Atomic Ions, Part I. Wavelengths*, NSRDS-NBS 68, U.S. Gov. Print. Off., Washington.
Sauval, A. J. and Tatum, J. B.: 1984, *Astrophys. J. Suppl.* **56**, 193.
Sørensen, G.: 1976, in I. A. Sellin and D. J. Pegg (eds.), *Beam-Foil Spectroscopy I. Atomic Structure and Lifetimes*, Plenum Press, New York, p. 165.
Tsuji, T.: 1973, *Astron. Astrophys.* **23**, 411.
Tsuji, T.: 1997, private communication of 'current' values of coefficients.
Vaeck, N., Godefroid, M., and Froese Fischer, C.: 1992, *Phys. Rev. A* **46**, 3704.
Wasson, J. T.: 1985, *Meteorites: Their Record of Early Solar System History*, Freeman, New York.
Wasson, J. T. and Kallemeyn, G. W.: 1988, *Phil. Trans. R. Soc. London* **325A**, 535.
Whiting, E. E.: 1973, *NASA Tech. Note* D-7268.