Analysis of the $3d^6 4s(6D) 4f - 5g$ supermultiplet of Fe I in laboratory and solar infrared spectra

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ABSTRACT

The combined laboratory and solar analysis of the highly-excited sub-configurations $3d^6 4s(6D) 4f$ and $3d^6 4s(6D) 5g$ of Fe I has allowed us to classify 87 lines of the $4f - 5g$ supermultiplet in the spectral region 2545-2585 cm$^{-1}$. The level structure of these JK-coupled configurations is predicted by semiempirical calculations and the quadrupolic approximation. Semiempirical gf-values have been calculated and are compared to gf values derived from the solar spectrum. The solar analysis has shown that these lines, which should be much less sensitive than lower excitation lines to departures from LTE and to temperature uncertainties, lead to a solar abundance of iron which is consistent with the meteoritic value ($A_{Fe} = 7.51$).

Subject headings: atomic data, line: identification, sun:spectra

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1. Introduction

The spectrum of Fe I is a significant opacity source in spectra of the sun and cool stars, and recent studies have illustrated the importance of highly excited configurations in the infrared spectrum of the sun. On the basis of a laboratory Fourier Transform (FT) spectrum Biémont et al. (1985) published a list of ~1200 iron lines between 1 µm and 4.1 µm that corresponded to lines in the solar spectrum. Roughly 300 of these lines had been identified in FT spectra by Litzén and Vergès (1976), and another 370 were observed in a very recent study of highly excited configurations in Fe I (Nave & Johansson 1993). The 3d⁶4s⁶⁵⁷g subconfiguration was established from 4d – 4f transitions by Johansson & Learner (1990), which resulted in the identification of about 200 solar lines in the atmospheric windows between 1.4 µm and 2.1 µm.

In this paper we present the analysis of the 3d⁶4s⁶⁵⁷g subconfiguration of Fe I that has been established by transitions to the 3d⁶4s⁶⁵⁷g levels (Johansson & Learner 1990) using laboratory FT spectra. Since the excitation energies of the 3d⁶4s⁶⁵⁷g and 3d⁶4s⁶⁵⁷f subconfigurations are only 0.5 to 0.8 eV lower than the ionization energy, 7.9 eV, these very high excitation lines of Fe I provide important information about plasma conditions. Even if there are slight non-LTE effects in Fe I for levels of lower excitation energies (Blackwell et al. 1984), lines from high excitation levels should be formed in LTE and should be rather insensitive to slight temperature uncertainties. The 4f and 5g electrons do not significantly penetrate the 3d⁶4s core, and the positions of the 3d⁶⁵⁷d⁶⁵⁷⁴f and 3d⁶⁵⁷⁴f⁶⁵⁷⁵⁷g subconfigurations relative to the series limit can therefore be predicted. Both subconfigurations are best described in the JK coupling scheme. The 4f – 5g lines occur in a narrow region of 35 cm⁻¹ (0.056 µm), 100 cm⁻¹ to the blue of the Br α(4 – 5) line of hydrogen at 2467.75 cm⁻¹ (4.05 µm). This region is shown in Fig. 1.

The presence of 4f – 5g lines in ground-based IR spectra of the sun and of α Tau (Ridgway et al. 1984) was first reported by Johansson et al. (1991). Most of the high resolution infrared atlas of the solar spectrum have been obtained from ground-based observations, and in some regions the telluric contribution totally obscures the lines. The solar spectrum has been recently obtained with the ATMOS space experiment (Farmer & Norton 1989). It is completely free of telluric lines, and the high resolution and signal-to-noise ratio allow us to make a much more detailed analysis of the Fe I 4f – 5g lines. Preliminary results have already been given by Geller (1992), Johansson et al. (1993), and Schoenfeld et al. (1993a).

2. Laboratory Observations and Analysis

The laboratory spectrum used was recorded on the Fourier transform spectrometer at the National Solar Observatory, Tucson, and details of the experimental setup have been described elsewhere (Learner & Thorne 1988). The source was a hollow cathode of pure iron run in 3.7 Torr of neon and a DC current of 1.4 A. The wavenumber resolution is 0.012 cm⁻¹. The 4f – 5g transitions reported here are also present at a lower signal-to-noise on other FT spectrograms taken in this region. The better quality of the spectrogram used in the present study appears to be mainly due to water cooling of the cathode in the light source.

The spectra were reduced with the DECOMP program of Brault and Abrams (1989) to give the wavenumber, integrated intensity, width and damping parameter for each line. The spectra were wavenumber calibrated from 26 Ar II lines (Norlén 1973) present in our visible region spectra, and the calibration was carried into the infrared by using overlapping wide-range spectra (Nave et al. 1992). The calibration constant for the spectrum used in this study was less than 0.001 cm⁻¹. The strongest, unblended lines in the spectrum are determined with a precision of ~0.0005 cm⁻¹, but almost all of the 4f – 5g lines are blended. The uncertainty of weaker lines is given by the full width at half maximum divided by the signal-to-noise and can be as much as 0.008 cm⁻¹ for the weakest lines.

Both the 3d⁶⁵⁷⁴f⁶⁵⁷⁴f and 3d⁶⁵⁷⁴f⁶⁵⁷⁵⁷g subconfigurations are best represented in the JK coupling scheme (Johansson & Learner 1990). The gross structure within each subconfiguration is defined by the fine structure splitting of the 3d⁶⁵⁷⁴f⁶⁵⁷f term in Fe II. The energy levels are then split into pairs, and the distribution of the centres of gravity of the pairs is described by a quadrupole approximation, determined by the electrostatic parameter F⁵(3d, nl). If the centres of gravity are plotted against the scalar product h = Jc · l of the total angular momentum of the core Jc, and the orbital angular momentum of the outer electron l, a set of parabolas is obtained – one for each
value of $J_c$. As previously noted for the $^5D$ term of $3d^6$ (Johansson & Learner 1990), both bowl-shaped and umbrella-shaped parabolas are obtained. This is due to a change of the sign in the energy expressions for J-K-coupled subconfigurations built on particular Hund terms, which will be thoroughly discussed in a forthcoming paper (Schoenfeld et al. 1993b). The vertices of the parabolas are predicted to be at $h = -\frac{1}{4}$. In Fig. 2 we have fitted parabolas to the observed energy levels of $3d^64s(^6D)5g$. The experimentally determined vertices lie from $h = -0.01$ to 0.05, and the deviations of the energy levels from the parabolic curve are $\sim 0.02$ cm$^{-1}$. In the $3d^64s(^6D)4f$ subconfiguration the energy levels are, with one exception (see below), split into resolved pairs by the Coulomb exchange interaction, but in $3d^64s(^6D)5g$ the pair splittings are too small to be resolved. Values for each energy level of a pair have been determined from lines in which theoretical gf-values predict only one transition to be important.

The experimentally determined energy levels are given in Table 1. The majority have been determined from the laboratory line list presented in Table 2. However, a few energy levels with low J have not been found as the necessary lines were not present in our laboratory spectra. Calculated gf-values of lines from these levels imply that they would not be distinguishable from the noise. The positions of these “missing” energy levels have been predicted from the parabolas in Fig. 2 and the predictions agree with a quadrupole moment polarization theory (Schoenfeld et al. 1993a). Many lines from these predicted energy levels appear weakly in the solar spectrum, and this has enabled us to establish another three levels which are marked with the superscript ‘S’ in Table 1. The remaining two predicted levels are marked with the superscript ‘P’ and are given to two decimal places. Two decimal places are also given if both levels of a pair are determined by a line in the laboratory spectrum from which only one wavenumber is determinable. An example is the line at 2556.948 cm$^{-1}$ which is the only line determining the pair of levels $5g(\frac{9}{2}|\frac{15}{2})$. In this case neither the $4f$ nor $5g$ pair splitting can be resolved. If a level is determined from weak or blended lines, for which the wavenumbers are uncertain, it is also given to two decimal places (e.g. $5g(\frac{7}{2}|\frac{9}{2})$).

We have revised the energy levels of both $3d^64s(^6D)4f$ and $3d^64s(^6D)5g$ by using a least squares fitting program, and have connected them to the rest of the term diagram of Fe I by means of transitions to $3d^64s(^6D)4d$. The energy level values we have obtained for the $3d^64s(^6D)4f$ levels are systematically higher than those reported previously (Johansson & Learner 1991) by $\sim 0.004$ cm$^{-1}$, since the wavenumbers for $4d - 4f$ transitions in our other set of infrared laboratory spectra are also systematically higher than previously reported. We attribute this difference to the improved method of wavenumber calibration that we have used in the current spectra. Estimates of the accuracy of the levels are given in column 4 of Table 1, and range from 0.003 cm$^{-1}$ for levels determined from strong, unblended lines to 0.01 cm$^{-1}$ for levels determined from blended lines. Predicted levels are probably accurate to 0.05 cm$^{-1}$. However, it should be noted that these energy levels refer to one set of plasma and discharge conditions in a hollow cathode lamp, and deviations of several mK ($1mK = 0.001$ cm$^{-1}$) may be found when comparing them with data obtained under other operating conditions or from other light sources. For instance, a systematic shift of $\sim 0.006$ cm$^{-1}$ is observed between the laboratory and solar data used in this study, where the laboratory wavelengths are about 0.1 Å longer than the solar wavelengths. This is further discussed in Sec.3.

The similar arrangement of the energy levels in $3d^64s(^6D)4f$ and $3d^64s(^6D)5g$ means that all the $4f - 5g$ lines are concentrated into a narrow region from 2545 cm$^{-1}$ to 2580 cm$^{-1}$. Almost all of the laboratory lines in this region are due to this supermultiplet, and unblended lines have a consistent width of 0.045 – 0.050 cm$^{-1}$. All of the laboratory lines are also present in absorption in the ATMOS spectrum of the sun, as can be seen from Fig. 1. The identified $4f - 5g$ lines are presented in Table 2. Table 3 gives lines observed in the solar spectrum but not in our laboratory spectra that have been identified as $4f - 5g$ lines by using the energy levels of table 1. As previously mentioned, some of these are too weak to be distinguishable from the noise in the laboratory spectrum, but others are strong and are masked by neon lines.

The reliability of the identifications in Table 2 can be seen by comparing the intensities of lines measured in the laboratory and solar spectra (Fig. 3). The large scatter at low intensities suggests there are still unresolved blends or incorrectly fitted lines in both the laboratory and solar spectrum; we note also that the fit of the weakest solar lines is generally less
accurate than that for other lines. The points with the largest deviation correspond to regions where the blending is particularly severe (~2563.6 cm\(^{-1}\) and 2567.8 cm\(^{-1}\)). Points lying below the line indicate a blend with another iron line in the laboratory spectrum. Points lying above the line indicate blends in the solar spectrum and an example of such a blend with a Si line is marked. Moreover, the curve of growth effect, which is well visible in our strongest solar lines, clearly explains the non-linear relation between laboratory and solar intensities (see also section 3).

The ninth column of Table 2 gives log(gf) values for the 3d\(^6\)4s\((^3D)4f\) - 3d\(^6\)4s\((^3D)5g\) supermultiplet which have been calculated with the Cowan computer code (Cowan 1981). Most of them agree to within 1% with the hydrogenic gf-values calculated in the pure JK coupling scheme. The calculations predict that the strongest transitions are of the form \((J_e[K]J - (J_e+1)[K+1])_{J+1}\), and that no transitions with \(\Delta J_e \neq 0\) are expected. The few differences between the calculations and the hydrogenic gf-values can be traced to mixing between different 4f levels. For example, calculations predict that the 4f\((\frac{5}{2})\)\(\frac{5}{2}\) at 57152.412 cm\(^{-1}\) and 4f\((\frac{5}{2})\)\(\frac{7}{2}\) at 57154.265 cm\(^{-1}\) are mixed, and an examination of the 4f - 5g intensities suggests the designations of these two levels should be exchanged. This is confirmed by a better fit of the revised levels to the parabolic curve for the \(J_e = \frac{5}{2}\) levels of 4f. However, even if the designations are exchanged the calculated gf-values for all transitions involving these two levels are less reliable. This level mixing enables \(|\Delta K| = 2\) transitions to occur. For example, in Table 2 the line at 2567.683 cm\(^{-1}\) arises from K=3.5 \(\rightarrow\) 5.5, and in Table 3 the line at 2563.052 cm\(^{-1}\) arises from the K=1.5 \(\rightarrow\) 3.5 transition.

An example of mixing between a 4f level and another Fe I level is illustrated by 4f\((\frac{5}{2})\)\(\frac{5}{2}\) at 57431.116 cm\(^{-1}\), which is mixed with 3d\(^6\)4s\((^3D)6p\)\(\frac{5}{2}\) at 57437.192 cm\(^{-1}\). This results in a line at 2562.206 cm\(^{-1}\) due to the transition 6p\(^5\)P\(^2\) - 5g\((\frac{5}{2})\)\(\frac{5}{2}\). The transition 6p\(^5\)P\(^2\) - 5g\((\frac{7}{2})\)\(\frac{5}{2}\) contributes to the blend in the solar spectrum at 2563.52 cm\(^{-1}\) and is probably the reason for the fact that 4f\((\frac{5}{2})\)\(\frac{5}{2}\) - 5g\((\frac{5}{2})\)\(\frac{3}{2}\) is not observed. As this mixing is not predicted by calculations it is not possible to calculate gf-values for these transitions, and the calculated gf-values for transitions involving 4f\((\frac{5}{2})\)\(\frac{5}{2}\) may be too large.

### 3. Solar Analysis

Between 2545 and 2585 cm\(^{-1}\) more than ninety percent of the solar lines in the ATOMS infrared solar spectrum (Farmer & Norton 1989) are identified as Fe I 4f - 5g transitions. These relatively faint lines in the solar spectrum have profiles that are typical for highly-excited transitions: they are broad with very extended wings. They have almost Lorentzian shapes whereas profiles of faint, low-excitation lines are Gaussian.

Although faint, these 4f-5g lines are very sensitive to the damping constants. This was shown in Fig. 3 of Johansson et al. (1993), where we only considered broadening by collisions with hydrogen atoms, computed from the Unsöld (1955) approximation. This frequently used approximation should, in principle, be valid for these highly excited “hydrogenic” levels. We found, however, that the damping constant computed in this way was too small to reproduce the observed solar lines profiles. This is also the case for lines between levels of low excitation (see e.g. Blackwell et al. 1984; Holweger et al. 1991). As shown in Fig. 4, very good agreement is obtained between synthetic and observed line profiles when the collisional damping constant is multiplied by an enhancement factor of about 2.5.

Even if the broadening due to collisions with neutral particles increases tremendously with the excitation energy, the Stark broadening increases even more rapidly. For the relatively high excitation energy associated with the Fe I 4f - 5g lines, the Stark broadening (Chang & Schoenfeld 1991; Carlsson et al. 1992) is only about 1/3 of the Van der Waals broadening. For transition arrays at even higher excitation energies, e.g. the 5g - 6h lines of Fe I (Schoenfeld et al. 1993b), the Stark broadening becomes more important.

We have fitted synthetic line profiles to the observed solar spectrum in the region of the Fe I 4f - 5g lines between 2545 and 2585 cm\(^{-1}\) using the photospheric model of Holweger & Müller (1974), together with a microturbulent velocity of 1 km/s. An example of our fit is shown in Fig. 5, together with the relevant portion of the laboratory spectrum. We have used a solar iron abundance of \(A_{Fe} = 7.51\) (in the usual scale, \(A_{Fe} = \log(N_{Fe}/N_{H}) + 12.0\)), which is the meteoritic value (Anders & Grevesse 1989). Recent investigations by different authors (Holweger et al. 1990; Holweger et al. 1991; Biémont et al. 1991; Hannaford et al. 1992) have shown that the photo-
spheric abundance of iron agrees with the meteoritic value.

We have been forced to apply a somewhat larger Doppler correction to the solar $4f - 5g$ Fe I lines than in the case of CO lines (see Fig. 5 in Farrenq et al. 1991) and of low excitation Fe I lines. The solar wavenumbers of our $4f - 5g$ Fe I lines, which are given in the fifth column of Table 2, have been corrected by a total Doppler shift of 66 mK instead of about 60 mK as found for other low excitation solar lines. We are unable to attribute this additional shift of about 6 mK to conditions in the solar photosphere. It is more likely to be due to pressure shifts in the hollow cathode; calibration problems would also affect the low excitation lines (Nave et al. 1992). Stark shifts in the hollow cathode, which can be as large as 30 mK in certain lines of neon (Chang et al. 1993), are calculated to be less than 1 mK for the $4f - 5g$ lines of Fe I.

Our “astrophysical gf-values”, derived from the ATMOS solar spectrum and the meteoritic iron abundance, are given in the seventh column of Table 2. The best solar line profiles are marked by an asterisk in the last column. Some additional solar lines (such as Si I, CH and OH and other, as yet unidentified lines from Geller (1992)) were simulated through artificial metallic lines and fitted to the observations. “Astrophysical gf-values” for lines not present in the laboratory spectrum are given in the fifth column of Table 3 together with calculated gf-values in column 7.

Good agreement is found between solar-derived gf-values and the calculated gf values, as can be seen from Fig. 6 where $\log (gf)$ is plotted against the log of the calculated gf-value. Most of the points lie on a well-defined line, which proves the consistency of the set of calculated gf-values. Based on the best selected solar lines, the solar-derived gf values are systematically somewhat smaller than the calculated values by a mean amount of about -0.10±0.05 dex. Although this could be due to the adopted solar abundance of iron, the difference is more likely due to uncertainties both in the calculated and solar gf-values. The main uncertainties of our solar-derived gf-values are due to the adopted damping constants (which require a rather large enhancement factor of about 2.5) and to an uncertainty in our measured intensities (due to a possible error of a few percent in the zero intensity level and also to the difficulty of determining the true local continuum in the solar spectra). The discrepancy between solar and theoretical gf values quoted hereabove is the highest possible value obtained when adopting the lowest possible continuum value. Therefore the general agreement remains within all experimental and theoretical combined errors.

It is interesting to compare the $3d^64s(6D)4f$ - $3d^64s(6D)5g$ supermultiplet in Fe I with the $3s4f - 3s5g$ multiplet in Mg I, for which extensive solar atmosphere modelling has been carried out (Chang et al. 1992). There, the hundred or so lines in only one Fe I supermultiplet are reduced to a few blended lines in one $^1F - ^3G$ and one $^3F - ^3G$ multiplet in Mg I. The Mg line cores were found to be formed at a height of 350 km (above $\tau_{600}=1$). Since Mg and Fe have comparable ionization potential and abundance, the weaker Fe I lines are expected to be formed lower in the solar atmosphere. Our calculations show that the center of the strongest Fe $4f - 5g$ lines are formed at a height of ∼240 km, with the weaker lines formed deeper (∼175 km) in the solar atmosphere, at about the same height as the fainter Mg I lines (e.g. $5f - 7g$).

4. Conclusions

We have classified 87 lines of the Fe I $3d^64s(6D)4f$ - $3d^64s(6D)5g$ supermultiplet by combining laboratory and solar data with theory. We have established all but two of the 58 levels in the $3d^64s(6D)5g$ subconfiguration, 53 from laboratory FT spectra, and three from the solar spectrum. Both configurations are best described using the JK coupling scheme. All the classified lines strictly obey the $\Delta J = 0$ rule, but we have found some violations of the other rule, $|\Delta K| \leq 1$. These are caused by mixing of certain levels of the same $J_c$ and $J$, but of different $K$ in the $4f$ subconfiguration. Besides this level mixing, the $4f$ subconfiguration is also subject to configuration interaction with $3d^64s(6D)6p$, due to the accidental coincidence of $6p$ $^5P_2$ level and $4f$ ($^5\Pi$/$^7\Pi$)2. The 5g configuration is found to be in JK coupling without any mixing whatsoever.

All of the lines in the $3d^64s(6D)4f$ - $3d^64s(6D)5g$ supermultiplet that we have observed in the laboratory are also present in the solar spectrum and account for more than 90 % of the lines between 2545 and 2585 cm$^{-1}$. We have calculated semi-empirical gf-values for most of the identified lines and have compared these with gf-values derived from the solar spectrum. From these $4f - 5g$ lines, which we expect to be much less sensitive than lower excitation lines to de-
partures from LTE and to temperature uncertainties, we have determined a solar abundance of iron which is consistent with the meteoritic value \( A_{Fe} = 7.51 \).

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| designation<sup>a</sup> | J | Level<sup>b</sup> (cm<sup>-1</sup>) | Error (cm<sup>-1</sup>) |
|------------------------|---|-------------------------------|------------------------|
| (4.5)[8.5]             | 9 | 59335.73                      | .01                    |
| (4.5)[8.5]             | 8 | 59335.72                      | .01                    |
| (4.5)[7.5]             | 8 | 59331.269                     | .005                   |
| (4.5)[7.5]             | 7 | 59331.270                     | .004                   |
| (4.5)[6.5]             | 7 | 59329.645                     | .004                   |
| (4.5)[6.5]             | 6 | 59329.642                     | .004                   |
| (4.5)[5.5]             | 6 | 59329.892                     | .004                   |
| (4.5)[5.5]             | 5 | 59329.891                     | .003                   |
| (4.5)[4.5]             | 5 | 59331.286                     | .004                   |
| (4.5)[4.5]             | 4 | 59331.287                     | .004                   |
| (4.5)[3.5]             | 4 | 59333.255                     | .004                   |
| (4.5)[3.5]             | 3 | 59333.257                     | .004                   |
| (4.5)[2.5]             | 3 | 59335.316                     | .003                   |
| (4.5)[2.5]             | 2 | 59335.317                     | .005                   |
| (4.5)[1.5]             | 2 | 59337.081                     | .005                   |
| (4.5)[1.5]             | 1 | 59337.078                     | .005                   |
| (4.5)[0.5]             | 1 | 59338.255                     | .01                    |
| (4.5)[0.5]             | 0 | 59338.27                      | .01                    |
| (3.5)[7.5]             | 8 | 59717.941                     | .007                   |
| (3.5)[7.5]             | 7 | 59717.94                      | .01                    |
| (3.5)[6.5]             | 7 | 59717.084                     | .005                   |
| (3.5)[6.5]             | 6 | 59717.079                     | .004                   |
| (3.5)[5.5]             | 6 | 59716.793                     | .004                   |
| (3.5)[5.5]             | 5 | 59716.792                     | .003                   |
| (3.5)[4.5]             | 5 | 59716.936                     | .004                   |
| (3.5)[4.5]             | 4 | 59716.944                     | .004                   |
| (3.5)[3.5]             | 4 | 59717.325                     | .004                   |
| (3.5)[3.5]             | 3 | 59717.317                     | .004                   |
| (3.5)[2.5]             | 3 | 59717.764                     | .004                   |
| (3.5)[2.5]             | 2 | 59717.759                     | .004                   |
| designation | Level (cm⁻¹) | Error (cm⁻¹) |
|-------------|-------------|--------------|
| (3.5) | 59718.13 .01 |
| (3.5) | 59718.13 .01 |
| (3.5) | 59718.41P .05 |
| (3.5) | 59718.41P .05 |
| (2.5) | 59999.211 .007 |
| (2.5) | 59999.206 .004 |
| (2.5) | 60001.343 .004 |
| (2.5) | 60001.337 .004 |
| (2.5) | 60001.575 .004 |
| (2.5) | 60001.56 .01 |
| (2.5) | 60000.71 .01 |
| (2.5) | 60001.390 .006 |
| (2.5) | 60198.124 .01 |
| (2.5) | 60198.12 .01 |
| (1.5) | 60193.670 .007 |
| (1.5) | 60193.666 .005 |
| (1.5) | 60197.940 .006 |
| (1.5) | 60197.937 .003 |
| (1.5) | 60196.429 .007 |
| (1.5) | 60196.42 .01 |
| (1.5) | 60192.14S .01 |
| (1.5) | 60192.14 .01 |
| (0.5) | 60309.69 .01 |
| (0.5) | 60309.70 .01 |
| (0.5) | 60309.711 .006 |
| (0.5) | 60309.717 .005 |

a Levels are marked in JK notation: \((J_c)[K]\).

P Predicted level value (see text).

S Level value derived from solar spectrum.
| Ia | widthb | λairc | σtc | σsd | Ie | log(gf)d | δσec | log(gf)e | Transitionf | Commentsg |
|---|---|---|---|---|---|---|---|---|---|---|
| 1.0 | 56 | 39274.98 | 2545.456 | .462 | 1.98 | 0.11 | -3 | 0.16 | (4.5)[1.5]1*(4.5)[1.5]1 | * |
| 1.0 | 31 | 39256.54 | 2546.652 | .636 | 1.56 | -0.37 | 16 | -0.24 | (4.5)[1.5]2*(4.5)[1.5]1 | * |
| 2.0 | 81 | 39245.13 | 2547.392 | .392 | 2.60 | -0.67 | 9 | -0.52 | (4.5)[1.5]2*(4.5)[1.5]1 | * |
| 2.5 | 64 | 39227.14 | 2548.561 | .567 | 2.38 | 0.27 | 1 | 0.42 | (4.5)[1.5]2*(4.5)[1.5]1 | * |
| 4.8 | 59 | 39166.76 | 2552.489 | .486 | 4.97 | 0.34 | 3 | 0.44 | (4.5)[1.5]2*(4.5)[1.5]1 | * |
| 1.5 | 37 | 39147.83 | 2553.724 | .742 | 2.08 | 0.21 | 1 | 0.32 | (4.5)[1.5]2*(4.5)[1.5]1 | * |
| 5.4 | 47 | 39119.70 | 2555.560 | .563 | 6.78 | 0.85 | 1 | 0.94 | (1.5)[1.5]2*(1.5)[1.5]1 | bl. OH |
| 2.4 | 47 | 39116.28 | 2555.774 | .782 | 2.98 | 0.37 | 1 | 0.47 | (4.5)[1.5]2*(4.5)[1.5]1 | * |
| 1.8 | 37 | 39113.03 | 2555.996 | .996 | 2.95 | 0.37 | 1 | 0.46 | (4.5)[1.5]2*(4.5)[1.5]1 | * |
| 7.4 | 49 | 39101.86 | 2566.726 | .726 | 8.56 | 0.97 | 1 | 1.04 | (4.5)[1.5]2*(4.5)[1.5]1 | * |
| 38.2 | 56 | 39098.46 | 2566.948 | .947 | 18.5 | 0.99 | 2 | 1.26 | (4.5)[1.5]2*(4.5)[1.5]1 | * |
| 1.1 | 43 | 39089.30 | 2557.547 | .55 | 2.0 | 0.17 | 3 | 0.17 | (4.5)[1.5]2*(4.5)[1.5]1 | * |
| 3.4 | 65 | 39081.53 | 2558.056 | .05 | 5.16 | 0.63 | 0 | 0.63 | (4.5)[1.5]2*(4.5)[1.5]1 | * |
| 1.0 | 54 | 39059.73 | 2559.484 | .48 | 0.78 | -0.12 | -5 | -0.17 | (1.5)[1.5]2*(1.5)[1.5]1 | * |
| 1.2 | 46 | 39054.63 | 2559.818 | .82 | 3.18 | 0.40 | -3 | -0.35 | (4.5)[1.5]2*(4.5)[1.5]1 | * |
| 3.0 | 41 | 39020.17 | 2562.079 | .095 | 12.22 | 0.77 | 0 | 0.87 | (2.5)[1.5]2*(2.5)[1.5]1 | * |
| 8.0 | 45 | 39019.59 | 2562.117 | .127 | 0.85 | -1 | 1.01 | (2.5)[1.5]2*(2.5)[1.5]1 | * |
| 0.6 | 34 | 39018.24 | 2562.206 | .21 | 0.97 | -0.05 | 6 | 0 | (6)[1.5]P2*(2.5)[1.5]2 | |
| 2.7 | 82 | 39015.94 | 2562.356 | .349 | 2.23 | 0.31 | 15 | 0.31 | (2.5)[1.5]2*(2.5)[1.5]1 | * |
| 10.9 | 54 | 39099.81 | 2563.416 | .420 | 10.5 | 1.05 | 2 | 1.10 | (2.5)[1.5]2*(2.5)[1.5]1 | * |
| 6.2 | 43 | 38998.05 | 2563.532 | .52 | 4.12 | 0.59 | -11 | 0 | (2.5)[1.5]2*(2.5)[1.5]1 | * |
| 1.0 | 46 | 38996.23 | 2563.651 | .655 | 1.86 | 0.20 | 1 | 0.37 | (2.5)[1.5]2*(2.5)[1.5]1 | * |
| 8.1 | 47 | 38994.34 | 2563.776 | .779 | 11.4 | 0.87 | -5 | 0.97 | (2.5)[1.5]2*(2.5)[1.5]1 | * |
| 1.1 | 42 | 38993.15 | 2563.854 | .85 | 0.94 | -0.10 | -11 | 0.21 | (3.5)[1.5]2*(3.5)[1.5]1 | * |
| 1.6 | 43 | 38992.14 | 2563.920 | .90 | 2.09 | 0.25 | 8 | 0.27 | (3.5)[1.5]2*(3.5)[1.5]1 | * |
| 18.7 | 45 | 38979.21 | 2564.771 | .770 | 15.3 | 1.08 | -2 | 1.21 | (3.5)[1.5]2*(3.5)[1.5]1 | * |
| 2.7 | 47 | 38972.11 | 2565.238 | .238 | 5.06 | 0.61 | 1 | 0.61 | (4.5)[1.5]2*(4.5)[1.5]1 | * |
| 7.5 | 43 | 38970.59 | 2565.338 | .338 | 8.77 | 0.26 | -9 | 0.30 | (3.5)[1.5]2*(3.5)[1.5]1 | * |
| 1.0 | 42 | 38968.21 | 2565.495 | .500 | 1.33 | 0.05 | 0 | 0.25 | (3.5)[1.5]2*(3.5)[1.5]1 | * |
| 13.3 | 44 | 38966.47 | 2565.669 | .610 | 12.2 | 1.10 | 0 | 1.27 | (3.5)[1.5]2*(3.5)[1.5]1 | * |
| 3.2 | 53 | 38964.72 | 2565.724 | .723 | 2.45 | 0.08 | 6 | 0.07 | (3.5)[1.5]2*(3.5)[1.5]1 | * |
| 2.1 | 46 | 38955.22 | 2566.351 | .347 | 5.33 | 0.74 | 1 | 0.84 | (0.5)[1.5]2*(0.5)[1.5]1 | * |
Table 2—Continued

| Laboratory Data | Solar Data | Identification | Comments^8 |
|------------------|------------|----------------|-------------|
|                  |            |                | I^a width^b /mK | λ_{air} /Å | σ_l /cm\(^{-1}\) | \(σ_s\) /cm\(^{-1}\) | I /mK | log(gf)^d | \(δσ^e\) /mK | log(gf)^e | Transition^f | 4f | 5g |
| 0.4 38 38952.60 | 2566.523   | .530 13.3 0.57 | 1 0.72 (4.5)[3.5] 4 (4.5)[4.5]_5 | | | | | | | | |
| 8.1 51 38951.54 | 2566.593   | .582 -0.07    | 10 -0.22 (0.5)[3.5] 3 (0.5)[3.5] | | | | | | | | | |
| 6.4 49 38950.49 | 2566.662   | .66 6.68 0.85 | 1 0.94 (0.5)[3.5] 3 (0.5)[3.5] | | | | | | | | | |
| 3.0 47 38942.22 | 2567.207   | .209 3.90 0.11 | 0 0.61 (4.5)[3.5] 3 (4.5)[3.5] | | | | | | | | | |
| 2.1 47 38941.63 | 2567.246   | .30 0.76     | (3.5)[3.5] 3 (3.5)[4.5] | | | | | | | | | |
| 2.6 50 38937.99 | 2567.485   | .483 2.93 0.40 | 2 0.70 (3.5)[3.5] 3 (3.5)[3.5] | | | | | | | | | |
| 4.7 47 38935.97 | 2567.619   | .35 3.57 0.49 | 0 0.51 (3.5)[3.5] 3 (3.5)[3.5] | | | | | | | | | |
| 3.1 42 38935.01 | 2567.683   | .680 4.33 0.58 | 0 ... (3.5)[3.5] 3 (3.5)[5.5] | | | | | | | | | |
| 15.4* 37 38932.78 | 2567.829   | .830 9.23 0.66 | 2 0.88* (3.5)[3.5] 3 (4.5)[5] | bl. in lab | | | | | | | | |
| 1.1* 23 38932.16 | 2567.870   | .860 0.65 5 0.83 (2.5)[2.5] 3 (2.5) | | | | | | | | | | |
| 3.8* 66 38931.37 | 2567.922   | .92 2.50 0.33 | 0 0.56 (3.5)[3.5] 3 (3.5) | | | | | | | | | |
| 3.8* 98 38929.41 | 2568.052   | .060 3.25 0.45 | -0.23 (3.5)[3.5] 3 (3.5) | | | | | | | | | |
| 0.9 24 38926.95 | 2568.214   | .200 1.83 0.19 | -2 0.61* (3.5)[3.5] 3 (3.5) | | | | | | | | | |
| 1.7 38 38926.04 | 2568.274   | .280 2.10 0.22 | 0 0.20* (2.5)[2.5] 3 (2.5) | | | | | | | | | |
| 2.3 23 38922.75 | 2568.491   | .492 5.05 0.52 | 0 0.72 (4.5)[3.5] 4 (4.5) | | | | | | | | | |
| 2.7 47 38914.93 | 2569.007   | .011 2.93 0.40 | -4 0.45 (3.5)[3.5] 3 (3.5) | | | | | | | | | |
| 9.7 48 38910.56 | 2569.296   | .299 10.22 1.00 | -2 1.08 (3.5)[3.5] 3 (3.5) | | | | | | | | | |
| 2.5 43 38905.52 | 2569.629   | .625 2.63 0.35 | 5 0.93* (3.5)[3.5] 3 (3.5) | | | | | | | | | |
| 8.3 39 38903.47 | 2569.764   | .774 4.73 0.62 | -12 0.54* (3.5)[3.5] 3 (3.5) | bl. in lab | | | | | | | | |
| 2.1 43 38899.57 | 2570.021   | .024 3.28 0.45 | -3 0.55 (3.5)[3.5] 3 (3.5) | | | | | | | | | |
| 11.8 55 38898.19 | 2570.113   | .112 10.50 1.04 | 1 1.14 (2.5)[2.5] 3 (2.5) | | | | | | | | | |
| 13.1 57 38895.16 | 2570.313   | .313 10.15 1.00 | -2 1.15 (3.5)[3.5] 3 (3.5) | | | | | | | | | |
| 2.7 41 38891.58 | 2570.550   | .553 2.71 0.24 | -2 0.27 (4.5)[3.5] 4 (4.5) | | | | | | | | | |
| 2.7 41 38891.58 | 2570.550   | .141 0.19 0.20 | 1 0.20 (2.5)[2.5] 3 (2.5) | | | | | | | | | |
| 8.9 52 38884.60 | 2571.011   | .011 21.0 1.42 | 0 1.02 (3.5)[3.5] 3 (3.5) | | | | | | | | | |
| 16.9 54 38882.47 | 2571.152   | .153 13.5 0.44 | -2 0.59 (3.5)[3.5] 3 (3.5) | | | | | | | | | |
| 6.0 34 38873.56 | 2571.741   | .741 8.78 0.97 | 0 1.07 (1.5)[3.5] 3 (1.5) | | | | | | | | | |
| 4.0 53 38872.34 | 2571.822   | .82 4.01 0.57 | 1 0.68 (2.5)[1.5] 3 (2.5) | | | | | | | | | |
| 0.6 19 38865.90 | 2572.248   | .2 2.57 0.37 | 5 0.13 (2.5)[3.5] 3 (2.5) | | | | | | | | | |
| 14.1 33 38866.33 | 2572.882   | .884 8.77 0.92 | 1 1.15 (1.5)[3.5] 3 (1.5) | | | | | | | | | |
| 4.0 52 38852.39 | 2573.142   | .142 3.39 0.42 | 0 0.57 (4.5)[6.5] 3 (4.5) | | | | | | | | | |
| 1.5 50 38850.23 | 2573.286   | .285 1.75 0.20 | 2 0.20 (2.5)[3.5] 3 (2.5) | | | | | | | | | |
| 12.4 53 38827.83 | 2574.770   | .770 10.72 0.99 | 0 1.14 (4.5)[6.5] 3 (4.5) | | | | | | | | | |
| 5.8 44 38824.95 | 2574.961   | .962 6.43 0.72 | -1 0.82* (4.5)[4.5] 3 (4.5) | | | | | | | | | |
| 8.2 56 38821.81 | 2575.169   | .170 6.28 0.71 | -1 0.91 (4.5)[4.5] 3 (4.5) | | | | | | | | | |
| 2.8 35 38816.49 | 2575.522   | .519 4.11 0.51 | 3 0.66 (4.5)[6.5] 3 (4.5) | | | | | | | | | |
| Laboratory Data | Solar Data | Identification | Comments  \\
|----------------|------------|----------------|-----------
| $I^a$ | width$^b$ | $\lambda_{air}$ | $\sigma_l$ | $\sigma_s$ | I | log(gf)$^d$ | $\delta\sigma^c$ | log(gf)$^e$ | Transition$^f$ | 4f | 5g |  \\
| 0.2 | 45 | 38803.83 | 2576.363 | .359 | 4.80 | 0.58 | 5 | 0.67* | (4.5)[4.5][3] - (4.5)[4.5][4] | * |  \\
| 6.2 | 64 | 38800.84 | 2576.561 | .564 | 5.85 | 0.68 | -3 | 0.75 | (4.5)[4.5][6] - (4.5)[4.5][5] |  \\
| 2.2 | 46 | 38799.23 | 2576.668 | .663 | 3.02 | -0.17 | 11 | 0.00 | (2.5)[0.5][7] - (2.5)[1.5] |  \\
| | | 38799.23 | 2576.668 | . | 0.32 |  | 7 | 0.49 | (2.5)[0.5][7] - (2.5)[1.5] |  \\
| 15.6 | 53 | 38792.07 | 2577.143 | .143 | 12.18 | 1.06 |  | 0 | 1.20 | (4.5)[6.5][3] - (4.5)[7.5] | * |  \\
| 10.1 | 53 | 38770.95 | 2578.547 | .547 | 8.13 | 0.84 |  | 0 | 0.99 | (4.5)[5.5][5] - (4.5)[6.5] | * |  \\
| 4.0 | 45 | 38767.21 | 2578.796 | .796 | 5.08 | 0.61 |  | 0 | 0.68 | (4.5)[5.5][5] - (4.5)[5.5] | * |  \\
| 10.9 | 49 | 38737.93 | 2580.745 | .747 | 9.86 | 0.94 | -1 | 1.06 | (4.5)[5.5][5] - (4.5)[6.5] | * |  \\
| 5.0 | 48 | 38734.17 | 2580.996 | .994 | 5.94 | 0.68 | 2 | 0.72 | (4.5)[5.5][5] - (4.5)[5.5] | * |  \\
| 0.6 | 17 | 38713.34 | 2582.385 | .388 | 1.28 | -0.02 | -3 | -0.02 | (4.5)[5.5][5] - (4.5)[4.5] | bl. Si |  \\

$^a$Intensity in arbitrary units. An asterisk marks unresolved lines. In the case of unresolved multiple components (in laboratory and solar spectra), the total intensity of the blend is only given in the row relative to the first component.

$^b$Full width at half maximum of line in FT spectra. Units are mK (1mK = 0.001 cm$^{-1}$)

$^c$Difference between laboratory wavenumber and that derived from the energy levels in table 1.

$^d$log(gf) value derived from the solar line intensity (with the solar equivalent width I in mK).

$^e$Calculated log(gf) value. An asterisk marks mixed levels for which the calculation is unreliable.

$^f$The 3d$^6$4s$(^6D)$4f configuration has been abbreviated as 4f, and 3d$^6$4s$(^6D)$5g as 5g. Levels are given in JK notation: $(J_c)[K]$, where $J_c$ is the J value of the parent level.

$^g$An asterisk marks a good solar line profile. Blends with other solar lines are indicated.
Table 3
ADDITIONAL 4f – 5g LINES DERIVED FROM THE ENERGY LEVELS AND OBSERVED IN THE SOLAR SPECTRUM

| λ_{air} / Å | σ^a / cm^{-1} | σ_s / cm^{-1} | I / mK | log(gf)_s^b | δσ^c / mK | log(gf)_{c}^d | Transition^e | Comments^f |
|-------------|----------------|----------------|--------|-------------|-----------|--------------|-------------|------------|
| 39302.12    | 2543.698       | .690           | 0.86   | -0.17       | 8         | -0.13        | (4.5)[1.5]_2-(4.5)[2.5]_2 |
| 39142.79    | 2554.045       | .047           | 1.15   | 0.05        | -2        | -0.01        | (1.5)[3.5]_3-(1.5)[3.5]_3 |
| 39124.99    | 2555.214       | .224           | 1.51   | 0.17        | -10       | 0.11         | (1.5)[3.5]_3-(1.5)[3.5]_4 Ne |
| 39035.87    | 2561.043       | .053           | 0.98   | -0.02       | -5        | 0.00         | (1.5)[2.5]_3-(1.5)[2.5]_3 |
| 39032.65    | 2561.229       | .230           | 2.02   | 0.27        | -1        | 0.30         | (2.5)[3.5]_3-(2.5)[3.5]_3 |
| 39007.02    | 2562.916       | .908           | 2.42   | 0.35        | 8         | 0.43         | (2.5)[3.5]_3-(2.5)[3.5]_4 |
| 38945.30    | 2567.004       | .010           | 1.06   | -0.01       | -6        | -0.99*       | (2.5)[2.5]_2-(2.5)[1.5]_1 |
| 38945.24    | 2567.008       |                |        |             | -2        | -1.61*       | (2.5)[2.5]_2-(2.5)[1.5]_2 |
| 38812.82    | 2575.766       | .774           | 0.68   | -0.29       | -8        | -0.29        | (4.5)[6.5]_2-(4.5)[5.5]_6 |
| 38809.11    | 2576.017       | .015           | 0.85   | -0.09       | 2         | -0.09        | (1.5)[4.5]_5-(1.5)[4.5]_4 |
| 38874.28    | 2578.326       | .326           | 1.53   | 0.06        | 2         | 0.06         | (4.5)[4.5]_2-(4.5)[3.5]_3 |

^a Wavenumber and wavelengths derived from the energy levels in table 1.

^b log(gf) value derived from solar spectrum.

^c Difference between wavenumber in solar spectrum and that in column 2.

^d Calculated log(gf) value. An asterisk marks mixed levels for which the calculation is unreliable.

^e The 3d^64s(^6D)4f configuration has been abbreviated as 4f. 3d^74s(^6D)5g as 5g. Levels are given in JK notation: (J_c)[K], where J_c is the J value of the parent level.

^f An asterisk marks a good solar line profile. ‘Ne’ indicates the line is masked by a neon line in the laboratory spectrum.
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Figures

1. Region of $4f - 5g$ transitions in Fe I. The upper section gives the solar spectrum (in absorption), and the lower section the laboratory spectrum (in emission). The two broad lines at 2555.13 cm$^{-1}$ and 2562.78 cm$^{-1}$ in the laboratory spectrum are neon lines. Some of the stronger $4f - 5g$ lines are marked by dotted lines.

2. Partial energy level diagram of Fe I showing the $3d^64s^6(6D)4f - 3d^64s(6D)5g$ energy levels arranged in the JK coupling representation. The ordinate is $h = \frac{1}{2} \{ K(K+1) - J_c(J_c+1) - l(l+1) \}$. The curves are parabolas fitted to the observed energy levels (circles) for each value of $J_c$.

3. Comparison of observed solar equivalent widths and laboratory intensities for $3d^64s(6D)4f - 3d^64s(6D)5g$ lines. The point marked ‘bl. Si’ is a blend of a $4f - 5g$ line and a Si line in the solar spectrum.

4. Comparison of observed and calculated solar line spectra with enhancement factors of 2 (top), 2.5 (middle), and 3 (bottom) for the collisional damping constant. The effect of an increase of the enhancement factor is clearly seen in Fe I $3d^64s(6D)4f - 5g$ line profiles.

5. Section of the solar spectrum (top) with a fitted synthetic spectrum indicated by dashed lines. The laboratory spectrum is shown below. The majority of lines in this section are due to Fe I and, with a few exceptions, can be assigned to the $3d^64s(6D)4f - 3d^64s(6D)5g$ supermultiplet.

6. Comparison of calculated gf-values and gf-values derived from the solar spectrum for $3d^64s(6D)4f - 3d^64s(6D)5g$ lines. Only the best, unblended solar lines (marked * in the last column of table 2) are included.