A new multiplet table for Fe I

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ABSTRACT

We have recorded spectra of iron-neon and iron-argon hollow cathode lamps in the region 1700 Å – 5 µm (59 000 – 2000 cm$^{-1}$), with Fourier transform (FT) spectrometers at the National Solar Observatory, Tucson, Arizona, U.S.A. and Imperial College, London, U.K., and with a high resolution grating spectrograph at the National Institute of Standards and Technology, Gaithersburg, U.S.A. The uncertainty of the strongest lines in the FT spectra is <0.002 cm$^{-1}$ (0.2 mA at 3000 Å; 8 mA at 2 µm). Pressure and current-dependent shifts are <0.001 cm$^{-1}$ for transitions between low lying levels, increasing to 0.006 cm$^{-1}$ for transitions between the most highly excited levels. We report 28 new energy levels of Fe I and revised values of another 818 levels. We have identified 9501 lines as due to 9759 transitions in Fe I, and these are presented in the form of a new multiplet table and finding list. This compares with the ∼5500 lines due to 467 energy levels in the multiplet tables of Moore (1950, 1959). The biggest increase is in the near ultraviolet and near infra-red, and many of the new lines are present in the solar spectrum. Experimental log(gf) values are included where they are available. A further 125 unidentified lines due to Fe I are given. The tables are also available in computer-readable form.

Subject headings: atomic data, line: identification

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1. Introduction

Spectra of low charge states of iron play a significant role in solar and stellar spectroscopy due to the high cosmic abundance of iron. The atomic structure of the iron-group elements is complex, and departures from any pure coupling scheme result in a high density of lines in all wavelength regions. The number of identified iron lines in the solar spectrum exceeds that of any other element, and the prediction that many unidentified solar lines in the near ultraviolet and near infrared are almost certainly due to Fe I (Johansson 1987) has been recently verified (Nave & Johansson 1993b). An updated analysis of the spectrum of neutral iron, Fe I, has been a long-standing request from astronomers, along with the needs for more and better laboratory data for many other elements, as emphasised at several recent meetings (for example Smith & Wiese 1992, Grevesse & Noels 1993, and the contributions of Kurucz and Lambert in Leckrone & Sugar 1993). The development of laboratory light sources and the techniques of Fourier transform (FT) spectrometry and high resolution grating spectrometry have made it possible to record the spectrum with an accuracy and completeness not previously achievable. This has enabled us to extend the term system considerably and to identify many new lines in astrophysical spectra (Nave & Johansson, 1993a,1993b). It is now possible to present an analysis of the spectrum which fulfills many current demands of astronomy.

Despite their age, the Revised Multiplet Table of Moore (1959) and the Ultraviolet Multiplet Table (Moore 1950) (both of which we shall refer to as MT) remain among the most widely-used sources of data for users requiring extensive line lists of atomic spectra (Edlén & Martin 1988). This popularity is undoubtedly due to the accuracy with which Moore prepared them, the care with which she selected data to be included, and the convenient format in which the data are presented. However, modern astronomical observations supersede old ones in signal-to-noise ratio, resolution, wavelength accuracy and spectral wavelength coverage. The line-by-line analysis of solar and stellar spectra has been replaced by comparisons between synthetic and observed spectra. All this puts new demands and requirements on the atomic data needs, and extensions and revisions to the MT have become an urgent necessity. Extensions are particularly needed in the near ultraviolet, where many new lines have been identified since the publication of the UV tables, and the near infrared above 1.3 μm, which is not covered by the MT. Revisions of the MT are required in all wavelength regions, as the accuracy of many lines in the MT has been substantially improved in recent years. The requirements of astronomy now demand wavelengths to within 1 mÅ in the visible and ultraviolet, and 0.001 cm−1 in the infrared. The data in the MT do not fulfill these requirements— as a recent search for the antecedents of a weak Fe I line showed, some of the wavelengths quoted actually go back to measurements made over a hundred years ago (Learner, Davies & Thorne 1991).

In addition to the MT, Moore published three volumes of atomic energy levels (Moore 1971), which also became standard references for atomic spectra. These were updated for the iron-group elements by Sugar and Corliss in 1985 (hereafter AEL-SC). The table for Fe I in the AEL-SC incorporates the revised levels of Crosswhite (1975) and Litzén (1976) and contains a list of references to earlier work. Since 1985, revisions to the energy levels and extensions to the term system have been made by Johansson (1987), Brown et al. (1988), O’Brien et al. (1991), Zhu and Knight (1992); further extensions based on the spectra presented in the current paper have been published by Johansson and Learner (1990), Nave and Johansson (1993a,b), Nave et al. (1994), and Johansson et al. (1994). Biémont et al. (1985) have also compiled a list of Fe I lines in the infrared solar spectrum.

The most recent compilation of gf-values for the iron-group elements is by Fuhr, Martin & Wiese (1988). The table for Fe I includes gf-values for ~1950 lines, some of which have an uncertainty of only a few per cent. More recent measurements include those of O’Brien et al. (1991), Bard, Kock & Kock (1991), Kock, Kroll & Schnehage (1984), and Meylan et al. (1993). In total, roughly 2600 Fe I lines now have measured gf values. The majority of these are between 3000 Å and 1 μm, where almost half of the observed Fe I lines now have measured gf-values. In the region below 3000 Å this drops to only 20%, and there are very few lines above 1 μm with measured gf-values.

Many astrophysicists now use the calculations of semi-empirical gf values by Kurucz (1989), which are based on experimental energy levels such as the ones presented in the present study. The calculations have the advantage that they include significantly more lines than it is possible to measure in the laboratory,
many of which are important in analyses of Fraunhofer spectra of the sun and cool stars. The disadvantage of these calculations is that their accuracy cannot be estimated and is often poor, especially for weak lines that may be the lines of most interest in studies of the iron abundance in the sun.

In this paper we present the analysis of the laboratory spectrum of Fe I in the form of a new multiplet table. The analysis is based on both FT and grating measurements of iron-neon and iron-argon hollow cathode lamps in the region 1700 Å to 5 μm (58 800 – 2000 cm$^{-1}$). The precision of the wavenumbers obtained from an FT spectrometer is up to an order of magnitude better than that obtainable with a grating spectrometer, but we have also included Fe I lines which were present in only the ultraviolet grating spectra, in which the number of Fe I lines is significantly higher (Nave & Johansson 1993a). We present revised values for 818 energy levels and values of 28 new levels. These give 9759 identifications of 9501 lines, which have been ordered into 2785 multiplets. Experimental gf-values are also given where they are available. A further 125 unidentified lines due to Fe I are presented.

2. Experimental Details

The laboratory spectra used in this study were obtained using three different instruments: the f/55 IR-visible-UV FT spectrometer at the National Solar Observatory (NSO), Tucson, Arizona for the region 2000 cm$^{-1}$ to 35 000 cm$^{-1}$ (0.05–0.29 μm); the f/25 vacuum UV FT spectrometer at Imperial College, London, for FT spectra in the region 33 000 cm$^{-1}$ to 59 000 cm$^{-1}$ (3000–1700 Å); and the 10.7m grating spectrograph at the National Institute of Standards and Technology (NIST), Gaithersburg, for high-dispersion grating spectra above 30 770 cm$^{-1}$ (<3250 Å).

The light source used for the FT investigations was a hollow cathode lamp, run in either neon or argon. In addition to Fe I spectra, this source also gives spectra of Fe II and the neutral and singly-ionised spectra of the carrier gas used. The cathode was usually an uncooled open-ended cylinder of pure iron, 8 mm in bore and 35 mm long. The metal case of the lamp formed the anode. The running pressures were about 5 mbar of Ne or 4 mbar of Ar for the visible and IR observations, and 3–4 mbar of Ne for the UV observations. The currents ranged from 320 mA to 1.1 A. In general, Ne gave a better signal to noise ratio for Fe I except in the region 14 000 – 17 500 cm$^{-1}$ (7100 – 5700 Å), where the strong Ne lines raise the noise level in the spectrum. Argon-iron spectra were therefore used in this region and were also recorded in the region 17 500 – 35 000 cm$^{-1}$ (2857 – 5714 Å) to give an absolute wavelength calibration based on Ar II lines. One infrared spectrum was recorded with a water-cooled cathode as source and a higher current of 1.4 A. Survey spectra were taken out to 600 cm$^{-1}$ (16μm), but they showed hardly any Fe I lines because of the high noise level from the thermal infrared background.

The wavenumber, integrated intensity, width and damping of all lines in the FT spectra were obtained using Brault’s DECOMP program (Brault & Abrams, 1989), which fits a Voigt profile to each line. The wavenumber scale was calibrated from 26 Ar II lines in the visible (Learner & Thorne 1988), and the calibration was carried into the UV and infra-red using wide-range spectra (Nave et al. 1991, 1992). Deuterium and tungsten lamps were used for intensity calibration.

The Doppler widths (half width at half maximum) varied from around 0.012 cm$^{-1}$ at 5000 cm$^{-1}$ (0.05 Å at 2 μm) to around 0.12 cm$^{-1}$ at 50 000 cm$^{-1}$ (5 mÅ at 2000 Å). This corresponds to a Doppler temperature of about 2500 K; the source is however, not in thermal equilibrium, and the intensity distribution is generally quite different from that of astrophysical spectra. Lines emitted from levels of high excitation are also Lorentz broadened, so the observed line widths are often higher than this. The uncertainty of the wavenumber of each line is the sum of statistical and systematic errors. The statistical error is equal to the half width at half maximum divided by the signal-to-noise ratio (Brault 1987). For lines with a signal-to-noise of ~100 this varies from around 0.0002 cm$^{-1}$ (0.8 mÅ at 2 μm) in the infra-red to 0.001 cm$^{-1}$ (0.01 mÅ at 3000 Å) in the ultraviolet. The weakest lines in the spectra have a signal-to-noise of ~3, and the accuracy is then of the order 0.005 cm$^{-1}$ (0.02 Å at 2 μm) in the infrared and 0.05 cm$^{-1}$ (5 mÅ at 3000 Å) in the ultraviolet. The most important systematic errors are the calibration error for each spectrum which is of the order 0.001 cm$^{-1}$, and possible pressure or current-dependent shifts. The latter have been estimated at <0.001 cm$^{-1}$ for levels of low excitation, rising to ~0.006 cm$^{-1}$ for the highest excitation levels. A full description of the procedure, with details of the FT spectra used in the present investi-
Grating spectra have been recorded in the region $30\,770 – 58\,820\,\text{cm}^{-1}$ ($3250 – 1700\,\text{Å}$) using iron-neon and iron-argon hollow cathode lamps. The iron-neon hollow cathode was run in continuous mode with DC currents of $0.6–0.8\,\text{A}$ and a gas pressure of $\sim 1.3\,\text{mbar}$. The iron-argon hollow cathode was run in pulsed mode with peak currents of $\sim 100\,\text{A}$, pulse width of $70\,\mu\text{s}$ and frequency $100\,\text{Hz}$, and pressure of $\sim 0.3–0.4\,\text{mbar}$. The spectra were calibrated from Ritz wavelengths obtained from interferometrically-measured Fe II lines (Norlén, private communication), and the uncertainty in the grating wavelengths is approximately $3\,\text{mÅ} (\sim 50\,\text{mK} at 2500\,\text{Å})$. The grating spectra are being used in an extended and comprehensive analysis of Fe II (Johansson & Baschek 1988).

### 3. Identification of Lines from Known Levels

The procedure we have followed to identify Fe I lines is to compare wavenumbers of observed lines with wavenumbers derived from measured energy levels. We will call the latter ‘Ritz wavenumbers’. The energy levels we have used in identifying the lines were from AEL-SC (Sugar & Corliss 1985), Brown et al. (1988), O’Brien et al. (1991), together with those we have located in our recent investigations of Fe I (Johansson & Learner 1991, Nave & Johansson 1993a, Nave et al. 1994, Johansson et al. 1994). To minimise the spurious coincidences of observed wavenumbers and Ritz wavenumbers, it is important to have a set of energy level values that is both accurate and appropriate to the sources used (O’Brien et al. 1991). We have therefore revised the energy levels from the observed transitions in the FT spectra, using a least squares fitting program (Radziemski et al. 1972), in which each line was assigned a weight inversely proportional to the square of the wavenumber uncertainty.

The values of the revised energy levels are listed in Table 1. We have listed the terms in order of the energy of the lowest fine structure level of each term. With the exception of a few levels, which we have carefully checked, the values are within the estimated errors of those previously published. In addition, 28 new energy levels have been found that have not been published elsewhere, and these are marked with an asterisk beside the level value in column 4.

Many energy levels in Fe I cannot be adequately described in any particular coupling scheme. We have given LS designations to all the levels where no other coupling scheme is obvious in order to label them and to help identify which configurations are incompletely represented. JK designations have been assigned to levels due to the configurations $3d^{6}4s(6D)\,6d,\,4f,\,5g$ and $3d^{7}(4F)4f$. Abbreviated term designations are given in column 2. These are extensions of the term designations used in the MT and follow the convention established in earlier papers (Brown et al. 1988; Nave & Johansson 1993a). The term designations and abbreviations are discussed in detail in section 4.1. Nine of the levels could not be assigned to a configuration and are represented only by their energy level values.

The primary criterion for identification of the lines was coincidence between the observed wavenumber and the Ritz wavenumber derived from the energy levels in Table 1, taking into account the uncertainty of the wavenumbers, the uncertainty of the levels, and possible blended lines. In many cases more than one identification is possible, particularly in the ultraviolet where many of the lines were detectable only in the less accurate grating spectra. Further criteria were thus applied to verify the identifications. In the grating UV spectra, Fe I and Fe II lines could often be distinguished by their relative intensities in spectra obtained from pulsed and unpulsed hollow cathodes. The absorption data of Brown et al. (1988) were also helpful as they contain no Fe II lines. Comparison was also made with published line lists and atlases of the solar spectrum (Moore, Minnaert & Houtgast 1966; Moore, Tousey & Brown 1982, 1992; Pierce and Breckinridge 1973; Swenson et al. 1970; Livingstone and Wallace 1991; Geller 1992), where all Fe I lines are present but Fe II lines of high excitation are absent.

### 4. Term Structure and Transitions

The term structure of the iron-group elements is described in detail in Johansson and Cowley (1988) and specific details pertaining to Fe I are given in Brown et al. (1988), Johansson and Learner (1991), and Nave and Johansson (1993a). The majority of the Fe I levels belong to the two configuration systems $3d^{6}4snl$ or $3d^{7}nl$. Terms at low excitation energies belong to the subconfigurations $3d^{6}(M\,L)4s4l$ and $3d^{7}(M\,L)4l$, and are often fairly well described in the LS coupling scheme. Higher excitation terms are usually of the form $3d^{6}4s(6D)nl$ or $3d^{7}(4F)nl$ and are...
in intermediate or JK coupling. The strongest transitions occur within each system when the parent or grandparent term, $^M L$, in the subconfiguration is unchanged.

### 4.1. Notation of Terms

In the MT the spectroscopic terms were abbreviated, as it was not possible at that time to describe them by their full spectroscopic notations. Since that time the convention used for the abbreviations has become well established and is the one adopted in the AEL-SC. The convention labels the lowest even-parity LS term of multiplicity $M$ and orbital angular momentum $L$ as $a^M L$, the next lowest, $b^M L$ and so on (e.g. the lowest $^3F$ term is labelled $a^3F$, the next lowest $b^3F$ ...). The lowest odd-parity term is labelled $c^M L$ and the next lowest $d^M L$ and so on. We have kept to this convention for all the terms that are given in the MT, but it cannot in general be extended to higher terms. It is not consistent – for example the lowest $^3D$ term is labelled $a^3D$, but the next lowest is labelled $c^3D$ — and it is a useful designation only in LS coupling, which does not apply to highly-excited terms.

All of the known extremely-excited terms in Fe I with $n > 4$ are formed by adding a running electron to either the $3d^6 4s {^6}D$ term or the $3d^7 {^4}F$ term in Fe II. These two terms are called the ‘parent terms’. Addition of one electron to each of these parents give the subconfigurations $3d^6 4s({^6}D) nl$ and $3d^7({^4}F) nl$, and the abbreviations we have adopted are intended to indicate the parent of the subconfiguration. Terms of the form $3d^6 4s({^6}D) nl$ $^M L$ are abbreviated to the form $s^n Dnl$ $^M L$ and terms of the form $3d^7({^4}F) nl$ $^M L$ to $4Fnl$ $^M L$. Highly-excited terms with $n = 4$ which were not labelled by Moore belong to other parents and grandparents, and are of the form $3d^6({^M L'}) 4s4p(3P) ^M L$, $3d^6({^M L'}) 4s4p(1P) ^M L$, or $3d^7({^M L'}) 4p ^M L$. These have been given the abbreviations $L'sp{^M L}$, $L'sp{^M L}$ and $L'{^M L'}4p{^M L}$, respectively.

Many highly-excited configurations with $l \geq 3$ are best described in the JK coupling scheme rather than the LS coupling scheme. In Fe I this applies to the subconfigurations $3d^6 4s({^6}D)$ 6d, 4f, 5g, and $3d^7({^4}F) 4f$. In JK coupling the levels split into groups, and each group has as a parent the same fine structure level in Fe II (Johansson & Learner 1990). The J-value of this parent level ($J_c$) is coupled to the angular momentum $l$ of the running electron to give a resultant $K$, which is in turn coupled to the spin of the running electron to give the J-value of the level. In Fe I, $J_c$ and $K$ are half-integral and $J$ is, as usual, integral. The full notation is, for example, $3d^6 4s({^6}D_{J_c}) 4f$ $[K] J$. The notation we use for the abbreviated term designation is $s^n D_{J_c} 4f$ $[K]$, with similar designations for other JK coupled subconfigurations.

In the computer-readable file, $J_c$ and $K$ have been truncated to integers. For example, the two levels due to $3d^6 4s({^6}D_{3/2}) 4f[\frac{1}{2}]$ are referred to as $s^6 D_{4.5} 4f[5.5]$ in the printed version of the table, and $s6D4f[5]$ in the computer-readable version.

### 4.2. Transitions and Selection Rules

As a result of the mixed coupling in Fe I the only selection rules that can reliably be applied are $\Delta J = 0, \pm 1$ ($J = 0 \neq J = 0$) and change in parity (we do not see any parity forbidden lines in our laboratory spectra). However, the multiplets containing the strongest lines fall in the visible and follow traditional LS rules — the transitions are between levels of the same multiplicity, with $\Delta L = 0, \pm 1$ (but not $L = 0 \rightarrow L = 0$). Amongst these, the strongest lines are the ones involving the levels with the highest $J$ where the J-value changes in the same direction as the L-value — for example in multiplet $a^2D - z^2D$ (number 88 in table 2, or MT multiplet 15) the strongest lines correspond to J changing by -1 (sometimes called the ‘main diagonal’), with the strongest line being $J=5 \rightarrow J=4$. The next strongest are for $\Delta J = 0$ (sometimes called the ‘first satellites’), and the weakest for $\Delta J = +1$ (sometimes called the ‘second satellites’). These rules are not always apparent from our intensities in Table 2, especially for multiplets involving the lowest terms ($a^2D$ and $a^2F$) which may be affected by self absorption.

However, many multiplets do not follow LS rules, even if the levels are of relatively low excitation. Transitions are seen both between levels with different multiplicities and with $\Delta L > 1$. The former are sometimes called ‘intercombination lines’, ‘spin-forbidden lines’, or ‘intersystem lines’, and their presence indicates the breakdown of the LS model. In complex spectra like Fe I they may be as common and strong as spin-allowed transitions. Multiplets of intercombination lines may not contain all of the theoretically predicted transitions between the two terms, and the intensities are often irregular as they depend on the degree of mixing with levels of other multiplicities. For example, in multiplet $a^3H - z^3G$ (464, MT 168)
the strongest lines are $6 - 5$, $5 - 4$ and $5 - 5$. The $5 - 6$ line is not observed and the $6 - 6$ line is relatively weak. This multiplet is caused by mixing between the $z^3\tilde{G}^o$ term and the $z^3\tilde{G}^o$ term, and the intensities are similar to those observed in multiplet $a^2H - z^3\tilde{G}^o$ (465, MT 169). The lines to $z^3G^o$ are weak because there is no level with $J = 6$ in the $z^3\tilde{G}^o$ term with which it can mix. Some multiplets are seen in which the multiplicity changes by 4. An example is the multiplet $a^1G - w^6G^o$ (963, MT 517), in which both the upper term and the lower term are mixed. In many cases, and in particular for highly-excited levels, it is difficult to identify exactly the way in which the levels are mixed, and a particular level may be described as a combination of several different LS components which all contribute more-or-less equally.

In highly-excited levels, where the dominant LS component may contribute only 30%, the concepts of an LS term and a multiplet have in general no meaning. For the sake of consistency, we have arranged all the transitions into multiplets, assigning LS labels according to the largest LS component, but the majority of lines in the infra-red are better arranged into ‘allowed supermultiplets’ which consist of all the transitions between two subconfigurations built on the same parent term. These supermultiplets usually obey the rule $\Delta l = \pm 1$ (sometimes $\Delta l = 3$ transitions are observed), and one generally observes all the transitions in each supermultiplet. For example, the multiplets $n^7D^o - s^6D5d\overline{M}L$ (2347–2354, 2356 and 2357) are due to $5p - 5d$ transitions between terms having the parent term $3d^64s^4D^0$, and if most of the lines in multiplet $n^7D^o - s^6D5d\overline{G}$ (2347) are seen then lines of the same or greater intensity in multiplets $n^7D^o - s^6D5d\overline{G}$ (2348), $n^7D^o - s^6D5d\overline{F}$ (2349), $n^7D^o - s^6D5d\overline{D}$ (2350) and so on, should also be observed.

Highly-excited levels due to $3d^64s(6D)nl$ odd-parity subconfigurations combine with the $3d^7(^4F)4s$ subconfiguration as well as the $3d^64s^2$ configuration, and the $3d - nl$ transitions are seen in the same spectral region as the $4s - nl$ transitions because of the similar energy of the $3d$ and $4s$ electrons in the transition elements. These transitions can also be regarded as allowed supermultiplets, because a possible alternative notation for $3d^7(^4F)4s$ is $3d^64s(6D)3d$. For example, multiplet $a^3F - s^6D6p\overline{F}$ (165) is due to a $3d^64s(6D)3d - 3d^64s(6D)6p$ transition. The lines in multiplets of $3d - nl$ transitions often have irregular intensities due to the different coupling in the higher and lower subconfigurations.

In some cases, configuration interaction gives multiplets between terms with different parents - for example configuration interaction between $3d^64s(6D)5d$ and $3d^7(^4F)6s$ gives rise to the multiplet $n^7D^o - ^4F6s\overline{3F}$ (2355), which is a transition between the $3d^64s(6D)5p$ and $3d^7(^4F)6s$ subconfigurations. In rather rare cases, $\Delta l = 3$ transitions occur between terms of the same parent: the multiplet $a^5H - s^6D_{4.5}4f$ (516) involves transitions of the form $4s^2-4s4f$, which probably occur because of configuration interaction between $3d^64s^2$ and $3d^74s$.

5. Table of Multiplets

The new multiplet table for Fe I is given in table 2. If a line is present in the FT spectra, the wavenumber and intensity is taken from these spectra; otherwise it is taken from the grating spectra. The criteria for ordering the multiplets are the same as in the MT. Each group of multiplets consists of multiplets with the same lower term, and the groups are ordered in increasing energy of the lower term ($a^5D$, $a^3F$, $a^3F \ldots$). Within each group, the multiplets are ordered in increasing energy of the upper term ($z^7\tilde{D}^o$, $z^7\tilde{F}^o$, $z^7\tilde{P}^o \ldots$). It should be noted, however, that some of the multiplets of Fe I listed in the MT are not ordered according to these criteria, as Moore only adopted the criteria part way through the typing of the Fe I table. This means that the order of multiplets in Table 2 is not necessarily the same as in the MT. Within each multiplet the lines have been listed in wavelength order. This is partly so that the user can work systematically through a spectrum and multiplet, and also because the irregular intensities observed in many multiplets rendered less meaningful the ordering scheme used in the MT – where the main diagonal, first satellites, and second satellites are listed in order of decreasing $J$.

A more important difference between Table 2 and the MT is that we present all the multiplets in one large table, which we consider to be more convenient for the user. This means that it is impossible to retain the old multiplet numbers of Moore, which in any case did not extend to the infrared, where many of our new multiplets are to be found. Our new numbers are given in column 1 of table 2. The term designations are given in column 2, and underneath these designations are given the number of the multiplet in the MT, where one exists, with the usual prefix of ‘UV’
for multiplet numbers taken from the UV multiplet table (Moore 1950). We have indicated designations that have changed since the MT with an asterisk after the number in the MT. Column 3 gives the two J-values for the transition.

The decision as to what constitutes a multiplet is particularly awkward where the levels are better described by the JK coupling scheme rather than the LS coupling scheme. We have decided to group all lines due to the same fine structure level of the parent, \( J_c \), together. For example, in multiplet \( z^7D^o - s^6D_{4,5}6d \) (454) all upper levels have the same parent level, \( 3d^64s^6D_{3/2} \) in Fe II, but have different \( K \)-values. For this reason we have labelled every line in these multiplets with the abbreviated term designation, to avoid confusion between levels of the same \( J \)-value but different \( K \).

The intensity of the line is given in column 4. The intensities of lines in the FT spectra are the logarithms of the integrated intensities and are given to two decimal places. The intensities of lines observed only in grazing spectra are integers, which are on a different scale to the FT spectra and are visual estimates of the photographic blackening in the continuous hollow cathode spectra. Lines marked ‘d0’ are faint and diffuse, and those marked ‘d0?’ are hardly detectable from the background. Lines marked ‘b’ are broad, and those marked with an asterisk are blended with other unresolved lines. Where a line is not present in the continuous hollow cathode spectrum, the intensity has been taken from the pulsed hollow cathode and is given in italics in the printed version of table 2 and in brackets in the computer-readable version.

In the lower multiplets many lines are affected by self absorption or self reversal. Self absorption widens the line and reduces its intensity, but the wavenumber remains unaffected (Nave et al. 1991). Intensities and experimentally measured wavenumbers are given for all of these lines, but in almost all cases accurate \( gf \) values have been measured and should be used instead of the intensities. Self-reversed lines have a pronounced dip in the centre of the line profile, and neither intensities nor accurate wavenumbers can be measured. No intensities are given for self-reversed lines and the wavenumbers are Ritz wavenumbers. All the FT intensities have been corrected for the response of the spectrometers, but it was not possible to maintain a completely consistent scale throughout the whole spectral region covered by table 2 because spectra in different spectral regions were obtained under several different source conditions, which affect the relative intensities of the lines. Nevertheless the information is still useful because it can help in identifying lines in other sources, and in many cases it is the only alternative to a calculated \( gf \) value, which can sometimes be wrong by an order of magnitude.

The vacuum wavelength given in column 5 is derived from the measured wavenumber in column 8. Wavelengths and wavenumbers of self-reversed and masked (i.e. obscured by a much stronger line) lines are Ritz wavelengths and wavenumbers. The superscript to the wavenumber is a measure of its uncertainty, taking into account both the statistical and systematic errors described in section 2. The errors in wavenumbers of lines graded ‘A’ are estimated to be less than 0.005 \( \text{cm}^{-1} \), lines graded ‘B’ less than 0.01 \( \text{cm}^{-1} \), lines graded ‘C’ less than 0.02 \( \text{cm}^{-1} \), and lines graded ‘D’ greater than 0.02 \( \text{cm}^{-1} \). All known blended lines and all lines measured only in grazing spectra have been assigned the grade ‘D’. The wavelength uncertainty \( \Delta \lambda \) in Å is obtained from the wavenumber uncertainty \( \Delta \sigma \) in \( \text{cm}^{-1} \) by using the relation:

\[
\Delta \lambda = \frac{\Delta \sigma}{\sigma^2} \cdot 10^8 = \Delta \sigma \cdot \lambda^2 \cdot 10^{-8} \tag{1}
\]

and typical values are given in table 3.

The air wavelengths in column 6 for all lines above 2000 Å have been derived from the wavenumbers using the Edlén dispersion formula (Edlén 1966):

\[
\lambda_R(\text{air}) = \frac{10^8}{\sigma_R} \times \left(1 + \frac{8342.13 \times 10^{-8} + 15997}{3.89 \times 10^9 - \sigma_R^2} \right) \times \left(1 + \frac{240630}{1.3 \times 10^{10} - \sigma_R^2} \right)^{-1} \tag{2}
\]

which agrees to within 1 mÅ with more recent infrared measurements by Peck and Reeder (1972). Column 7 gives the difference between the observed wavelength and the Ritz wavelength in mÅ. To obtain the Ritz wavelengths, the differences in column 7 should be subtracted from the wavelengths in column 5 or 6. Column 9 gives the difference between the observed wavenumber and the Ritz wavenumber, and the Ritz wavenumbers should be determined in a similar way. A large discrepancy between the measured wavelength of a line graded ‘A’ and the Ritz wavelength is indicative of an unknown and unresolved
Table 3

Uncertainties in wavenumbers and wavelengths

| Grade | $\Delta \sigma$ (cm$^{-1}$) | 2000 Å | 5000 Å | 1 μm | 2 μm | 5 μm |
|-------|------------------|--------|--------|------|------|------|
| A     | < 0.005          | 0.2    | 1.25   | 5    | 20   | 125  |
| B     | < 0.01           | 0.4    | 2.5    | 10   | 40   | 250  |
| C     | < 0.02           | 0.8    | 5.0    | 20   | 80   | 500  |
| D     | > 0.02           | 0.8    | 5.0    | 20   | 80   | 500  |

blend. Lines which are known to be blended with other Fe I, Fe II, Ne or Ar lines are marked in column 13 with the species of the blended line. Lines which are obscured by a much stronger line are marked with an ‘M’ in column 13, together with the species of the stronger, masking line.

The wavenumbers of all lines are necessarily those emitted by the iron atom in a specific set of plasma conditions, and are not those of an isolated atom. A detailed discussion of possible wavenumber shifts is given in Learner & Thorne (1988). The majority of our lines with upper levels of low excitation (<6 eV) have a very small Lorentzian component to the line profile, and can thus be expected to be relatively free from wavenumber shifts. Lines graded ‘A’ emitted from upper levels of low excitation should be selected where the accuracy of the wavelength is of particular importance, and the best of these are listed in the three recently published tables of recommended wavelength standards (Learner & Thorne 1988, Nave et al. 1991, Nave et al. 1992). Lines originating from levels of high excitation are Lorentz broadened and may be subject to pressure shifts. A recent comparison of the $4f - 5g$ transitions observed in our spectra with those observed in the sun indicated that the solar wavenumbers were roughly 0.006 cm$^{-1}$ less than the laboratory wavenumbers, which is probably due to pressure or current-dependent shifts in the hollow cathode (Johansson et al. 1994). Another possible source of wavenumber shifts is unresolved or partly-resolved isotope structure. We have as yet seen no evidence for isotope structure in Fe I, although it is of importance in Fe II and Ni I (Rosberg, Johansson & Litzén 1992, Litzén, Brault & Thorne 1993).

Columns 10 and 11 contain the excitation potentials of the lower and upper levels of the transition respectively. These are given in eV in the printed version of table 2, and in eV and cm$^{-1}$ in the computer-readable version. Experimental gf values have been taken from various sources in the literature and are given in column 12 (Fuhr, Martin & Wiese 1990; O’Brian et al. 1991; Meylan et al. 1993, Johansson et al. 1994). We have not estimated the accuracy of these measurements, and the user is advised to consult the original references. In particular, we note that some publications lead to a solar abundance of iron which is slightly greater than the currently accepted value (Holweger et al. 1991). Other recent measurements of gf-values or lifetimes in Fe I include Kock et al. (1984), Blackwell et al. (1986), Bard et al. (1991), and Engelke, Bard & Kock (1993). We have not included calculated gf values for the lines, partly because of their uncertain accuracy, but also because they are likely to be re-calculated with the new levels included. Calculated gf values for Fe I can be found in the tables of semi-empirical gf values by Kurucz (1989) or Fawcett (1987). Although the absolute accuracy of these calculations is often rather poor, the relative accuracy of calculated gf values of lines within a single multiplet can be quite good (Fawcett 1987, Blackwell 1983). The calculations of the Opacity Project (Sawey & Berrington 1992) include multiplet oscillator strengths, which may be helpful in estimating gf values for lines due to highly-excited levels that have not been measured or calculated by other groups.

Table 4 is a finding list for all the lines in table 2. For all lines above 2000 Å we give an air wavelength, $\lambda_{air}$, a wavenumber, $\sigma$, and the number of the multiplet in table 2 where the line can be found. We have only given vacuum wavelengths $\lambda_{vac}$ below 2000 Å, as in the air region they can easily be obtained from
the wavenumber of the line:

\[ \lambda_{\text{vac}}(\text{Å}) = 10^8 / \sigma(\text{cm}^{-1}) \]  

Table 5 gives 125 of the strongest unidentified lines in our spectra with a signal-to-noise ratio greater than 100. These are all probably due to Fe I, as they are present in either the solar spectrum or the absorption spectra of Brown et al. (1988). Some of these lines may well be due to the unclassified levels in Brown et al. (1988), but we have been unable to confirm them. The rest are probably due to highly-excited levels that we have been unable to find.

6. Fe I lines not listed in the table

The MT contains lines and multiplets that are not listed in table 2. Many of these lines have not been observed in any laboratory spectra, but are lines predicted from energy levels for which the Ritz wavelength coincides with a feature in the solar spectrum. They are designated in the MT by the symbol \( \odot \) in the intensity column and the letter ‘P’ in the reference column. As we do not see them in our spectra, we are unable to say whether all these lines are in fact due to Fe I. The Ritz wavelengths in the MT were based upon old energy level values, and more accurate wavelengths for them can be determined from the energy levels listed in table 1, provided that the identifications are correct and are unchanged. The Ritz wavenumber, \( \sigma_R \) in \( \text{cm}^{-1} \), is given by the difference between the upper and lower level values of the transition, and the Ritz vacuum wavelength in Å can be calculated from equation 3. To obtain the Ritz air wavelength \( \lambda_R(\text{air}) \), the Edlén dispersion formula in equation 2 should be used (Edlén 1966).

Ritz wavenumbers and wavelengths for all Fe I lines are also listed in the calculations of semi-empirical \( g_f \) values by Kurucz (1989), and use of Kurucz’s list has the advantage that calculated \( g_f \) values are also given, which would assist in judging whether a particular solar or stellar line is due to Fe I or not. It should be emphasised, however, that the wavelengths listed in Kurucz’s calculations will only be correct for energy levels that have been determined experimentally. This means that reliable wavelengths of lines will only be found in the smaller linelists distributed by Kurucz. The larger linelist also contains lines due to energy levels that have been calculated by atomic structure computer programs, and the wavelengths of these lines may be wrong by several Å or more, depending on the wavelength and accuracy of the calculations. The larger linelist should only be used when the details of the spectrum are unimportant (e.g. for opacity and radiation transport calculations) and it cannot be used for high-resolution spectroscopy.

Two other publications also contain lists of Fe I lines that are not present in table 2. Brown et al. (1988) have analysed the absorption spectrum of Fe I in the range 1550 Å to 3215 Å. Roughly 800 of the 3000 lines they observed are below 1700 Å, and fall outside the region of table 2. Between 1700 Å and 3215 Å they also observed many lines which are not present in our spectra. These are due to highly-excited odd-parity levels which are not well populated in a hollow cathode, but combine strongly with the ground term and consequently give strong lines in an absorption spectrum. Brown et al. (1988) list roughly 100 of these highly-excited levels. In the infra-red, Schoenfeld, Chang & Geller (1993) have identified two supermultiplets in the region of 3900 \( \text{cm}^{-1} \) (2.56 \( \mu \text{m} \)) and 1350 \( \text{cm}^{-1} \) (7.41 \( \mu \text{m} \)) due to \( 3f^54s^2(^6D) \) \( 4f \) \( - \) \( 6g \) and \( 3f^54s^2(^6D) \) \( 5g \) \( - \) \( 6h \) respectively, which have been observed in the solar spectrum. They also identify several features at longer wavelengths which are due to higher Rydberg transitions. All but the \( 4f \) \( - \) \( 6g \) supermultiplet are outside the range of our emission spectra, and this supermultiplet is not present due to the high excitation energy of the \( 6g \) levels.

7. Summary

The total number of energy levels in table 1 is 846, of which 28 are new. In comparison, the total number of energy levels from which the lines in the MT are derived is 467. Many of the new energy levels are of high excitation and are likely to be particularly useful in the interpretation of astrophysical spectra. The total number of lines in table 2 is 9501, which are due to 9759 transitions arranged into 2785 multiplets. This compares with the \( \sim \)5500 lines in the MT, of which roughly 1650 are Ritz wavelengths of lines present in the solar spectrum, but not observed in laboratory spectra. The biggest increase is in the ultraviolet below 3000Å, where the number of lines has increased from \( \sim \)750 to \( \sim \)2000, and in the infrared above 1\( \mu \text{m} \), where none of the \( \sim \)3000 lines in table 2 were given in the MT. The strongest lines have an uncertainty of \( <0.002 \text{ cm}^{-1} \) (0.2 mA at 3000 Å and 8 mA at 2 \( \mu \text{m} \)), which is up to an order of magnitude...
better than wavelength standards derived from previous data (Nave et al. 1991). Almost all of the lines are present in the solar spectrum, and in many cases correspond to strong lines.

Table 5 gives a good indication of the current state of the analysis of Fe I. Almost all of the strongest lines in the visible have been identified. In spite of the many new identifications in the infrared, the largest proportion of unidentified lines fall between 1 and 2 \( \mu m \). In the near UV, both our FT and grating spectra contain many unidentified lines, many of which are also strong unidentified lines in the solar spectrum. At present, no laboratory spectra of sufficient quality beyond 5.4 \( \mu m \) have been recorded, and it is not possible for us to estimate the contribution of Fe I to stellar spectra in this region. Table 2 also shows that relatively few lines in the infrared beyond 1 \( \mu m \) and few lines in the ultraviolet below 3000 Å have measured \( gf \) values. With the current interest in both ultraviolet and infrared astronomy they will almost certainly be required for stellar and solar spectroscopy.

Many users will prefer to have the new multiplet table in computer-readable form. For the time being, ascii versions of tables 1 and 2 are available by anonymous FTP from ferrum.fysik.lu.se (130.235.92.170) at Lund University, in the directory pub/iron. The ascii version of table 2 is also available sorted in wavelength order.

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