Wavelengths of Fe II lines for studies of time variation of the fine-structure constant

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ABSTRACT

Ritz wavelengths of 27 spectral lines of Fe II have been obtained from energy levels derived from Fourier transform spectra. The lines selected are observable in absorption spectra from quasi-stellar objects and are important for astronomical tests of the invariance of the fine-structure constant on a cosmological time-scale. By comparing the wavelength calibration in this paper with that of previously published measurements, wavelengths for 21 lines of Mg II, Mg II, Cr II, Ti II, Mn II, Ni II and Zn II have been placed on a scale consistent with the Fe II Ritz values.

Key words: atomic data – ultraviolet: general.

1 INTRODUCTION

The universality and constancy of the laws of nature rely on the invariance of the fundamental constants. However, some recent measurements of quasar (quasi-stellar objects, QSO) absorption line spectra suggest that the fine-structure constant, α, (Mohr, Taylor & Newell 2008) may have had a different value during the early Universe (Murphy, Webb & Flambaum 2003). Other measurements (e.g. Chand et al. 2006) appear to show no change. The attempt to resolve these discrepancies can probe deviations from the standard model of particle physics and thus provide tests of modern theories of fundamental interactions that are hard to attain in other ways.

QSO absorption lines are used in these investigations to measure the wavelength separations of atomic lines in spectra of different elements – the many-multiplet method (Dzuba, Flambaum & Webb 1999) – and compare the separations at large redshifts with the separations today. Any difference in the separations would suggest a change in α. This method requires very accurate laboratory wavelengths to be used successfully, since the changes in α reported by Murphy et al. (2003) are only a few parts in 10^7 or better (Berengut et al. 2009). Improved accuracy in measuring possible changes in α can be achieved by using many different lines from a variety of elements and species. However, it is vital that the laboratory wavelengths for all spectral lines used are on a consistent and accurate wavelength scale. There have been several measurements of atomic wavelengths using Fourier transform (FT) spectroscopy (Griesmann & Kling 2000; Pickering et al. 2000; Aldenius 2009; Ruffoni & Pickering 2010) made to increase the number and accuracy of atomic lines usable to detect changes in α. The status of these measurements has been summarized by Berengut et al. (2009), who also present a list of atomic lines for which better laboratory data are needed.

A previous paper (Nave & Sansonetti 2011) has made a detailed analysis of the wavelength scale of published Fe II lines and suggested corrections necessary to put these measurements on the scale of recent wavelengths derived from FT spectroscopy (Whaling et al. 1995), laser spectroscopy (Salit et al. 2004) and frequency comb spectroscopy (Hannemann et al. 2006; Salumbides et al. 2006; Batteiger et al. 2009). In Nave & Sansonetti (2011), we re-analysed the spectra used in the previous publications (Learner & Thorne 1988; Nave et al. 1994; Nave, Johansson & Thorne 1997a). These consisted of 31 FT spectra of iron–neon and iron–argon hollow cathode lamps covering wavelengths from about 1500 Å to 5 μm (66 000 to 2000 cm^-1). Measured wavelengths for the lines of the 3d(4p)4s a^2D–3d(4p)4f γ^2P multiplet were presented. This multiplet contains a line at 1608.45 Å that is particularly important for detecting changes in α as its variation with α has the opposite sign to that of other nearby lines (Murphy et al. 2003). However, many of the lines of interest for detecting possible changes in α have wavelengths below the current short-wavelength limit of FT spectroscopy. Wavelengths of these lines were previously measured using grating spectroscopy and have uncertainties more than an order of magnitude greater than the uncertainty required for measuring possible changes in α (Johansson 1978). In addition to the measured wavelengths in Nave & Sansonetti (2011), we optimized the values of 939 energy levels of Fe II using measured wavenumbers of 9567 measured lines. Some of these were used to derive Ritz wavelengths (i.e. wavelengths derived from optimized energy levels) for the a^2D–γ^2P lines. The optimized energy levels can also be used to derive Ritz wavelengths for lines below the limit of FT spectroscopy. This paper presents Ritz wavenumbers and wavelengths for lines of interest for detecting possible changes in α. A paper presenting the full list of energy levels and measured wavenumbers and wavelengths is in preparation.

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2 EXPERIMENTAL DATA AND ANALYSIS

The spectra used are the same as those used in previous studies of Fe I and Fe II (Learner & Thorne 1988; Nave et al. 1991, 1994, 1997a), and details of the experiments can be found in those papers. Three different spectrometers were used: the f/60 IR–visible–UV FT spectrometer (FTS) at the National Solar Observatory (NSO), Kitt Peak, Arizona, the f/25 vacuum ultraviolet (VUV) FTS at Imperial College, London (Thorne et al. 1987) and the f/25 VUV spectrometer at the National Institute of Standards and Technology (NIST) (Griesmann et al. 1999). The light sources for all of the spectra were high-current hollow cathode lamps containing a cathode of pure iron run in either neon or argon. Gas pressures of 100–500 Pa (0.8–4 Torr) were used with currents from 0.32 to 1 A. Roughly 28 000 lines were measured in 31 spectra, covering wavelengths from about 1470 Å to 5 μm (68 000 to 2000 cm⁻¹) at resolutions from 0.01 cm⁻¹ in the IR region to 0.08 cm⁻¹ in the VUV. The wavenumber, intensity and width for all the lines were obtained with Brault’s DECOMP program (Brault & Abrams 1989) or its modification XGREMLIN (Nave, Sansonetti & Griesmann 1997b). Each line was measured in between one and nine different spectra and weighted average values of the wavenumber, intensity and width were calculated.

The spectra were calibrated with lines of Ar II taken from Whaling et al. (1995), and details of this calibration are given in Nave & Sansonetti (2011). The calibration based on Ar II lines agrees with the calibration based on lines of Mg I and Mg II measured with a frequency comb (Hannemann et al. 2006; Salumbides et al. 2006; Batteiger et al. 2009) to better than 1×10⁻⁴.

The 28 000 lines were identified by comparison to previously published wavelengths in Ar I–II, Ne I–III, various lines of impurities present in the spectrum, and to Ritz wavelengths calculated using 947 energy levels of Fe II and 850 levels of Fe I (Nave et al. 1994). The Fe II levels included 576 levels from Johansson (1978), which are the most relevant for the Ritz wavenumbers presented in this paper, and additional unpublished levels. Roughly 10 000 lines matched energy level differences in Fe II. About one-third of these lines had more than one possible identification. The identifications of all known lines were checked to ensure that very few spurious identifications contributed to the energy level optimization, as even a small number of mis-identified lines can have a significant effect on the optimized energy levels. This task was aided by the small uncertainty of the wavenumbers obtained from a FTS, previous publications of the Fe I spectrum (Nave et al. 1994), and by predicted intensities from the atomic structure calculations of Kurucz (2010). Although the accuracy of these calculations is limited by strong configuration interaction in Fe II, they were useful for locating lines in FTS data from levels that had been found using less accurate data from grating spectographs. After eliminating spurious identifications, the total number of Fe II lines was 8930, of which 798 had more than one plausible identification.

The uncertainty of the wavenumbers measured in a single spectrum consists of the statistical uncertainty in the measurement of the position of the line and a calibration uncertainty for the whole spectrum. Part of the calibration uncertainty is derived from the uncertainty in the original standards and is common to all spectra. A further complication occurs when wavenumbers from many spectra are used to derive optimized energy levels, as the uncertainty of the energy levels depends on the calibration uncertainties of lines measured in different spectra covering wide wavelength regions. So the calibration uncertainty contributes to the uncertainty of the energy levels in two ways: as a contribution to the level optimization and as an overall calibration uncertainty for all wavelength regions. In these cases, it is impossible to perform a statistically rigorous level optimization. The approach used omits the calibration uncertainty during the optimization of the energy levels and combines the resulting energy level uncertainties in quadrature with a global calibration uncertainty. This ensures that the calibration uncertainty does not enter twice into the final Ritz wavenumber uncertainties.

The line uncertainties (one standard uncertainty) assigned for use in the level optimization omit the calibration uncertainty and were determined as follows. The statistical uncertainty was estimated from the full width at half-maximum of the line divided by twice the signal-to-noise ratio. This was derived from equation (9.3) of Davis, Abrams & Brault (2001), assuming roughly four statistically independent points in a linewidth. For lines measured in several spectra, a weighted average wavenumber and uncertainty was calculated using the reciprocal of the statistical uncertainty as a weight. The uncertainty was added in quadrature to a minimum estimated uncertainty of 0.001 cm⁻¹. This value was chosen to ensure that the level optimization is not dominated by the IR region, where narrow linewidths give very precise wavenumbers, but the uncertainty of the wavenumbers is higher than these lines are far from the Ar II calibration standards.

The measured lines were used to derive optimized energy levels and Ritz wavenumbers using the LOPT computer program (Kramida 2011). Values for 942 energy levels of Fe II were derived using 8930 lines covering wavenumbers from 2008 to 67 851 cm⁻¹. Weights were assigned proportional to the squared reciprocal of the estimated uncertainty of the wavenumber of the line. Lines with more than one possible classification, lines that were blended, and lines with a large difference between the observed and Ritz wavenumber were assigned a low weight.

Two iterations were made. In the first, lines connecting the lowest a⁰D term to higher 3d⁶(⁰D)⁴p levels were assigned a weight proportional to the squared reciprocal of the statistical uncertainty of the wavenumber, omitting the minimum estimated uncertainty of 0.001 cm⁻¹. This was done to obtain accurate values and uncertainties for the a⁰D intervals. These intervals are determined from differences between lines close to one another in the same spectrum sharing the same calibration. Hence the calibration uncertainty does not contribute to the uncertainty in the relative values of these energy levels. In the second iteration, the a⁰D levels were fixed to the values and uncertainties determined from the first iteration. The weights of all transitions were assigned by combining in quadrature the statistical uncertainty and the minimum estimated uncertainty of 0.001 cm⁻¹ in order to obtain accurate uncertainties for the 3d⁶(⁰D)⁴p and higher levels. The final level uncertainties with respect to the ground term are obtained from the LOPT program by combining the uncertainties derived from the level optimization in quadrature with a global calibration uncertainty of 4×10⁻⁸ times the level value.

3 RESULTS AND COMPARISON WITH PREVIOUS MEASUREMENTS

The Ritz wavenumbers and vacuum wavelengths derived from the optimized energy levels are presented in Table 1. Since the lower level of all the spectral lines is the ground level, the Ritz wavenumbers are the same as the level values and the wavenumber uncertainties are the same as the level uncertainties with respect to the ground level.
Previous FT spectroscopy measurements of accurate wavelengths for detection of possible changes in the fine-structure constant include Pickering et al. (2000), Griesmann & Kling (2000), Aldenius, Johansson & Murphy (2006) and Ruffoni & Pickering (2010). All four studies used Ar II lines as either the primary wavenumber standard or as confirmation of a scale based on other lines. However, differences in the values of the standards used and in the way in which the calibration was extended from the visible region to the UV result in small differences in the wavenumber scales of these studies. Since some of these studies have lines in common, it is possible to compare their wavenumbers to each other, and to the wavenumbers in this paper, in order to put all of these measurements on a common wavenumber scale. These comparisons are summarized in Table 2.

Six of the first seven lines of Table 1 have been measured previously by Aldenius et al. (2006), who reported wavelengths of Mg II, Mg II, Ti II, Cr II, Mn II, Fe II and Zn II lines measured simultaneously in a hollow cathode discharge using FTS. Her Fe II wavenumbers agree with the Ritz wavenumbers within the joint uncertainties, but are 3.7 parts in 10⁶ smaller (Nave & Sansonetti 2011). All her wavenumbers should be increased by 3.7 parts in 10⁶, and her wavelengths decreased by the same factor, to put them on the same scale as the Ritz wavenumbers in Table 1. These revised wavenumbers are given in column 4 of Table 2. The excellent agreement of her recalibrated wavenumbers with those from the frequency comb and from Nave & Sansonetti (2011) suggests that the uncertainty of the recalibrated wavenumbers is significantly better than the uncertainty given in table 1 of her paper. This is consistent with the fact that the dominant contributor to the uncertainty of her strong lines was the uncertainty in the calibration. A revised estimate of the uncertainty of her recalibrated lines can be obtained by combining her estimated statistical uncertainty of 0.0005 cm⁻¹ with the uncertainty in the revised calibration of 3 × 10⁻⁹ times the wavelength (Nave & Sansonetti 2011). These uncertainties are given in column 4 of Table 2. The uncertainties of her Mn II lines and of the Fe II line at 2260.779 Å have not been revised, as they appear to be dominated by the statistical uncertainties rather than the calibration.

Pickering et al. (2000) report wavelengths of Cr II, Zn II and Ni II lines measured using FTS. Their spectra were calibrated from 17 lines of Fe II taken from Nave et al. (1991). Nave & Sansonetti (2011) show that the wavenumbers of the Fe II lines in Nave et al. (1991) are 10.6 parts in 10⁶ smaller than the Ritz wavenumbers reported here. Hence all the wavenumbers in Pickering et al. (2000) should be increased by 10.6 parts in 10⁶, and the wavelengths decreased by the same factor, to put them on the same scale as the Ritz wavenumbers and wavelengths in Table 1. These revised wavelengths are given in column 5 of Table 2. Pickering et al. (2000) estimate the uncertainty of their measurements to be less than 0.001 cm⁻¹ when calibration

<table>
<thead>
<tr>
<th>Upper level¹</th>
<th>Ritz wavenumber²</th>
<th>Ritz vacuum wavelength²</th>
<th>Previous vacuum wavelength²</th>
</tr>
</thead>
<tbody>
<tr>
<td>3d(4D)⁴p²D₈/₃₂</td>
<td>38458.3928(17)</td>
<td>2600.17210(11)</td>
<td>2600.17223(10)</td>
</tr>
<tr>
<td>3d(4D)⁴p²D₅/₃₂</td>
<td>38660.0528(17)</td>
<td>2586.64934(11)</td>
<td>2586.64957(10)</td>
</tr>
<tr>
<td>3d(4D)⁴p⁴F₁/₁₂</td>
<td>41968.0679(20)</td>
<td>2382.76397(11)</td>
<td>2382.76441(10)</td>
</tr>
<tr>
<td>3d(4D)⁴p⁴F₉/₇₂</td>
<td>42114.8372(19)</td>
<td>2374.46009(11)</td>
<td>2374.46014(10)</td>
</tr>
<tr>
<td>3d(4D)⁴p²F₇/₅₂</td>
<td>42237.0563(19)</td>
<td>2367.58924(11)</td>
<td>2367.5878(10)</td>
</tr>
<tr>
<td>3d(4D)⁴p⁴F₇/₅₂</td>
<td>42658.2440(19)</td>
<td>2344.21776(11)</td>
<td>2344.21282(10)</td>
</tr>
<tr>
<td>3d(4D)⁴p²D₇/₅₂</td>
<td>44232.5393(20)</td>
<td>2249.87547(10)</td>
<td>2249.875(10)</td>
</tr>
<tr>
<td>3d(4D)⁴p²D₇/₅₂</td>
<td>44446.9044(19)</td>
<td>2249.87547(10)</td>
<td>2249.875(10)</td>
</tr>
<tr>
<td>6d(3F)⁴p²F₃/₁₂</td>
<td>62065.5273(5)</td>
<td>1611.20037(7)</td>
<td>1611.201(5)</td>
</tr>
</tbody>
</table>

¹The lower level of all the lines is the ground level 3d⁶(1D)⁴s⁴D₈/₃₂.
²The uncertainty in the last digit(s) of the wavenumber and wavelength is given in parenthesis.
³References: (t) Aldenius (2009); (t) Nave & Sansonetti (2011); (t) Nave et al. (1997a); (t) Johansson (1978) Ritz values; (t) Green (1939); (t) Dobbie (1938). Uncertainty estimates in parenthesis are from the original papers if given.
Table 2. Comparison of revised vacuum wavelengths between this and previous work.\textsuperscript{a}

<table>
<thead>
<tr>
<th>Species</th>
<th>Frequency comb</th>
<th>This work</th>
<th>Aldenius (2009)\textsuperscript{b}</th>
<th>Pickering et al. (2000)\textsuperscript{c}</th>
<th>Ruffoni &amp; Pickering (2010)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Mg \textsuperscript{i}</td>
<td>2852.962794(16)\textsuperscript{d}</td>
<td>2852.96272(9)</td>
<td>2852.96280(10)</td>
<td>2852.96270(6)</td>
<td></td>
</tr>
<tr>
<td></td>
<td>2026.474983(3)\textsuperscript{e}</td>
<td>2026.47496(6)</td>
<td>2026.47500(8)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Mg \textsuperscript{ii}</td>
<td>2803.530981(5)\textsuperscript{f}</td>
<td>2803.53102(9)</td>
<td>2803.53119(10)</td>
<td>2803.53095(6)</td>
<td></td>
</tr>
<tr>
<td></td>
<td>2796.353789(5)\textsuperscript{f}</td>
<td>2796.35393(9)</td>
<td>2796.35397(10)</td>
<td>2796.35387(5)</td>
<td></td>
</tr>
<tr>
<td>Fe \textsuperscript{ii}</td>
<td>2600.17210(11)</td>
<td>2600.17214(9)</td>
<td>2586.64934(11)</td>
<td>2586.64928(9)</td>
<td></td>
</tr>
<tr>
<td></td>
<td>2382.76397(17)</td>
<td>2382.76402(8)</td>
<td>2374.46004(8)</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>2344.21276(99)</td>
<td>2344.21273(8)</td>
<td>2260.7793(3)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Cr \textsuperscript{ii}</td>
<td>2066.16383(7)</td>
<td>2066.16381(6)</td>
<td>2056.25675(7)</td>
<td>2056.25671(6)</td>
<td></td>
</tr>
<tr>
<td>Ti \textsuperscript{ii}</td>
<td>3384.72989(12)</td>
<td>3384.72981(12)</td>
<td>3242.91789(11)</td>
<td>3230.12160(11)</td>
<td></td>
</tr>
<tr>
<td>Mn \textsuperscript{ii}</td>
<td>2606.45873(20)</td>
<td>2606.45873(20)</td>
<td>2594.49659(20)</td>
<td>2576.87524(20)</td>
<td></td>
</tr>
<tr>
<td>Ni \textsuperscript{ii}</td>
<td>1751.9155(1)</td>
<td>1741.5529(1)</td>
<td>1709.6040(1)</td>
<td>1703.4117(4)</td>
<td></td>
</tr>
<tr>
<td>Zn \textsuperscript{ii}</td>
<td>2062.66032(4)</td>
<td>2062.66032(4)</td>
<td>2026.13689(6)</td>
<td>2026.13698(4)</td>
<td></td>
</tr>
</tbody>
</table>

\textsuperscript{a}Uncertainties in last digit(s) given in parenthesis.
\textsuperscript{b}Wavelengths decreased by 3.7 parts in 10\textsuperscript{−8}. Uncertainties have been revised as in Section 3.
\textsuperscript{c}Wavelengths decreased by 10.6 parts in 10\textsuperscript{−8}. Uncertainties have been revised as in Section 3.
\textsuperscript{d}Salumbides et al. (2006).
\textsuperscript{e}Hannemann et al. (2006).
\textsuperscript{f}Batteiger et al. (2009).

4 CONCLUSIONS

Ritz wavenumbers and wavelengths for 27 lines of Fe \textsuperscript{ii} of potential use for detection of changes in \(\alpha\) have been derived from FTS measurements of iron hollow cathode lamps. The uncertainty of the wavenumbers is between 3 \times 10\textsuperscript{−5} and 1.7 \times 10\textsuperscript{−4}\textdegree. The wavenumber scale has been derived from Ar \(\text{ii}\) wavenumbers and is consistent with the scale based on frequency comb measurements of Mg \(\text{i}\) and Mg \(\text{ii}\).

The scale has been compared to that used in previous publications of lines of relevance for measurement of variations in the value of \(\alpha\) (Pickering et al. 2000; Aldenius 2009; Ruffoni & Pickering 2010). By recalibrating the wavelength scale used in these publications, wavelengths of 48 lines of Mg \(\text{i}\), Mg \(\text{ii}\), Ti \(\text{ii}\), Cr \(\text{ii}\), Mn \(\text{ii}\), Fe \(\text{ii}\), Ni \(\text{ii}\) and Zn \(\text{ii}\) have all been placed on a consistent scale.

Acknowledgments

This work was partially supported by NASA inter-agency agreement NNH10AN38I.
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