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Comprehensive atomic wavelengths, energy levels and hyperfine structure for singly-ionized iron-group elements.

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Abstract

We summarize recent work at the National Institute of Standards and Technology and Imperial College London on wavelengths, hyperfine structure, energy levels, and analysis of singly-ionized iron-group elements of astrophysical interest.

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FIG. 1: Top panel: Black line shows spectrum of HD 175640 adapted from Fig. 4 of Castelli et al. [1]. Red line shows the synthetic spectrum including the high-excitation lines of Mn II marked with vertical red lines. Bottom panel: Laboratory spectrum of Mn-Ne hollow cathode lamp. The strong line at 238.54 nm in both spectra is due to the new energy level $3d^5(^6S)6d^5D_4$

I. INTRODUCTION

Spectral lines of singly-ionized iron-group elements are observed in a wide variety of astrophysical objects including A- and B- type stars, the interstellar medium, quasi-stellar objects, and in absorption spectra from quasi-stellar objects. Although lines of Fe II, Cr II and Ni II often dominate these spectra, relatively low abundance iron-group elements such as Sc II can also be important as their abundance can be significantly higher in some objects. Even high-excitation energy levels, which give rise to few spectral lines in laboratory atomic spectra, can be of importance in interpreting stellar spectra. Figure 1 shows lines of Mn II with upper levels at about 12.5 eV to 14 eV present in the star HD 175640 [1]. The laboratory spectrum of a manganese hollow cathode lamp (hcl) shows only the strongest lines as the upper levels of these transitions are not well populated in the light source. In the absorption spectrum of the star, only the lower level needs to be populated, so transitions to higher levels are observed more easily. This indicates that almost all Mn II lines seen in laboratory data are of potential importance for line identification in stellar spectra. In order to understand these spectra it is thus necessary to obtain and analyze high-resolution, high signal-to-noise ratio laboratory spectra to obtain accurate wavelengths and energy levels for all of the singly-ionized elements from scandium through nickel.

For many years, the atomic spectroscopy groups at the National Institute of Standards and Technology (NIST), USA and Imperial College London (ICL), UK, have been recording and analyzing high-resolution spectra of iron-group elements using Fourier transform (FT) and grating spectroscopy. In 2012 NIST and ICL joined forces in order to complete the analysis of singly-ionized spectra from scandium through nickel using high-resolution Fourier transform and grating spectroscopy. The combined wavelength region of our measurements extends from 82 nm to 5000 nm and covers the region of almost all of the allowed lines of astrophysical interest from these elements. Hyperfine structure parameters are being measured using our FT spectra.

II. EXPERIMENTS

Our spectra are recorded using three high-resolution FT spectrometers and a normal incidence vacuum spectrograph (NIVS). Archival data from these spectrometers and from the National Solar Observatory digital archive [2] of spectra from the Kitt Peak FT spectrometer are also used where available. The NIST 2-m FT spectrometer covers wavelengths from 300 nm to 5500 nm at a limiting resolution as small as 0.0025 cm^{-1} , sufficient to resolve the Doppler width of the spectral lines from the typical sources we use for this work. At shorter wavelengths, two vacuum ultraviolet (UV) FT spectrometers at NIST and ICL [3] cover wavelengths from 140 nm to 900 nm at a limiting resolution as small as 0.025 cm^{-1} . Although FT spectrometers provide excellent wavelength precision and resolution, the sensitivity of FT spectrometers in the UV is lower than that obtained with a grating spectrometer with a photographic plate or image plate detector. Our FT spectra are thus supplemented with spectra from our 10.7-m NIVS at NIST, covering the region 82 nm to 350 nm with a resolution of about 0.0017 nm. Although the wavelengths from this instrument have a higher uncertainty than those from our FT spectrometers, we typically record over twice as many lines in the region of overlap using our NIVS.

The sources used for our spectra are high-current water-cooled hollow cathode lamps. The lamp used at NIST is the design of Danzmann et al. [4], operating in neon, argon or helium at currents of up to 2 A. It can be used without a window on our NIVS in the region below 110 nm. A similar lamp is used at ICL at currents of 600 mA to 1000 mA.

III. WAVELENGTH CALIBRATION

The high density of spectral lines in iron-group spectra mean that accurate and precise wavelengths are essential for reliable line identification. The wavenumber scale of FT spectrometers is linear to better than $1:10^7$ and in principle can be calibrated with only one wavenumber standard, although more are typically used [5]. This accuracy is sufficient for most astrophysical applications. More stringent requirements for the wavenumber scale are demanded by the studies of quasar absorption line spectra for investigating possible changes in the fine structure constant α during the history of the Universe [6], where wavenumber uncertainties of just 0.001 cm^{-1} can be statistically significant. This has resulted in several studies using FT spectrometry aimed at providing accurate wavelengths for these investigations [7–11]. All of these studies used visible-region lines of Ar II as calibration standards [5, 12], with the wavelength calibration extended to the UV region using overlapping spectra. However, inconsistencies in the wavenumber standards used, and problems in extending the wavenumber scale to the UV region, resulted in small discrepancies between the wavelength scales of these studies which become important for the precision measurements required to look for changes in α . The key to reconciling these studies was the availability of precise measurements of Mg I and Mg II lines using frequency comb spectroscopy [13–15], providing reliable wavelength standards in the UV with an uncertainty of roughly $1.5:10^9$ at wavelengths as low as 203 nm. This enabled us to reconcile the wavelength scales and put all of the measurements on a consistent scale [16].

To obtain wavelength standards at shorter wavelengths than can be achieved with FT spectroscopy, Ritz wavelengths based on energy levels optimized using FT spectra can be generated. Using this technique, we have extended our wavelength standards in Fe II to 105 nm, obtaining uncertainties of the order of $5 \times 10^{-5} \text{ nm}$ near 105 nm [16]. Additional standards in Si II and Fe I with similar uncertainties have been derived using the same method [17]. Accurate and precise values for these short wavelengths are particularly valuable as they enable the study of changes in the fine structure constant at higher redshifts using the high resolution of astronomical spectrographs operating in the visible region.

FIG. 2: Energy level structure of Mn II

IV. TERM STRUCTURE OF THE IRON-GROUP ELEMENTS

Figure 2 shows the energy level structure of Mn II, and is representative of the structure of other singly-ionized iron-group elements. A more detailed description of the structure of these elements is given in [18]. The terms can be grouped into three systems. The first is of the form $3d^k$. The second, referred to as the singly-excited system by [18], takes the form $3d^{k-1}nl$. The groups of terms follow the structure of the $3d^{k-1}$ parent terms of the doubly-ionized atom. The doubly-excited system takes the form $3d^{k-2}4s nl$, with terms following the structure of the $3d^{k-2}$ parent terms in the trebly-ionized atom. As can be seen from Fig. 2, the energy difference between the 4s and 4p terms, and between the 4p and 5s terms is similar for all levels based on the different parent terms. This results in a dense spectrum in the UV region from 200 nm to 300 nm due to strong 4s-4p transitions based on each of the parents. Transitions between different levels belonging to different parents are much weaker. For most elements the terms based on the lowest parent in the singly-excited system are the most complete and may extend up to $3d^{k-1}5g$ levels or higher. Many of the levels based on higher parents in both systems have yet to be found as they are not well populated in a hollow cathode lamp. Lines from these levels may still appear in absorption in stellar spectra, where the lower level rather than the upper level needs to be populated for the line to appear.

After wavelength calibration all spectra from both the FT spectrometers and grating spectrograph are merged into a single linelist. Lines corresponding to known transitions in the carrier gas of the lamp (He, Ne, or Ar), the neutral or doubly-ionized species of the element, or other impurities are identified using previous analyses.

Although the processes of identifying the singly-ionized lines in such a spectrum is simply a matter of comparing the differences between known levels and the measured wavenumbers, this is difficult in practice for complex atomic spectra. A typical combined linelist of both FT and grating spectra may contain over 30 000 spectral lines, with over a third of them due to the singly-ionized atom. The number of energy levels in such a species may be over 1000, so the probability of a spurious coincidence between an energy level difference and an observed line is high, particularly if the energy level values were determined from older and less accurate grating measurements. Hence the first step in the analysis is to start with a small number of identified lines, improve the level values, and then add in successively more lines and levels until all the level values have been improved. We are using the program LOPT [19] for this level optimization. Care needs to be taken to ensure that only reliable line identifications are used in the optimization, as even one blended line or spurious identification can affect the optimization of all of the level values. Comparison with semi-empirical atomic structure calculations, such as those of Kurucz [20], can aid in eliminating such spurious identifications. However, the process can be particularly problematic when putting terms based on higher parents on the same energy scale as those based on the lowest parent, particularly if the multiplicity of the parents are different. Lines linking these terms are likely to be weak. Their oscillator strengths are rarely calculated accurately by atomic structure calculations. They only appear due to interactions between LS terms from different parents and these interactions cannot be calculated accurately. Even with energy levels optimized to high-accuracy spectra many spurious coincidences will occur. Experience is thus required as the calculations are not sufficiently accurate for reliable identification.

After identifying as many of the lines as possible using the known energy levels, a search can be made for additional levels using the unidentified lines in the list. These are likely to be high-excitation levels where the principal quantum number $n \geq 5$. The most fruitful place to look for these levels is the infrared (IR) region using transitions of the form $nl - (n+1)(l+1)$. The narrow linewidths and high accuracy of IR FT spectra means that small tolerances can be used in the search for new levels, greatly reducing the number of spurious

FIG. 3: Increase in the number of identified lines in Fe II of Nave & Johansson [21] over Johansson [22]

levels found. Once such levels have been found in the IR, additional lines in the UV can be identified using transitions from the new levels to the ground and other low-excitation terms. Hence the principal improvement to be made in the identification of new spectral lines is in the UV and IR regions, as can be seen for Fe II in Fig. 3 for the recent analysis of [21].

Hyperfine structure (HFS) is an additional complication in the analysis of complex spectra. HFS constants are not known for many levels of iron-group elements, but are essential in the modeling of stellar spectra in order to obtain accurate abundances. Figure 4 shows a section of the HgMn star HD175640, showing two Mn II lines where the HFS constants of the upper level were known, but not the constants for the lower level. A new analysis of archival laboratory data to obtain the HFS constants explains the discrepancy between the stellar spectrum and the synthetic spectrum [23].

V. CURRENT STATE OF ANALYSIS

The following section summarizes the current state of analysis of singly-ionized iron-group elements.

Sc II The most recent published analysis was by Johansson & Litzén [25] and covered the

FIG. 4: A comparison of the observed spectrum of HD 175640 with the synthetic spectrum of Castelli & Hubrig [24] (red) in the region of the $3d^5(^4D)4s b^5D_3 - 3d^5(^6S)4p z^5P_2$ (940.70 nm) and $3d^5(^4D)4s b^5D_2 - 3d^5(^6S)4p z^5P_2$ (940.86 nm) transitions. The new positions of the HFS components are shown in blue [23]

wavelength region 110 nm to 1100 nm. Hyperfine structure parameters for 16 levels were subsequently published by [26]. We have measured new FT spectra covering the region 180 nm to 2200 nm and the analysis is in progress.

Ti II An unpublished analysis of Ti II based on FT spectroscopy, covering wavelengths from 180 nm to 2200 nm, was recently incorporated into a NIST compilation [27]. About 100 lines below 180 nm in this compilation were taken from older grating measurements [28] and have an uncertainty of 0.002 nm. We have taken spectra with our NIVS that have a wavelength uncertainty roughly an order of magnitude lower. They show many more lines, particularly in the region below 136 nm that was poorly covered in the older measurements. Identification of these lines will require new analysis of FT spectra.

V II An analysis of this spectrum based on FT spectroscopy between 149 nm and 2900 nm was published by Thorne et al. [29]. At shorter wavelengths, the most recent work is by the group of Iglesias ([30] and references therein). We plan additional grating measurements to reduce the wavelength uncertainty at these short wavelengths by more

than an order of magnitude and identify new lines using the levels of [29]. Hyperfine structure constants for 55 levels were determined from fast ion beam laser spectroscopy by Armstrong et al. [31].

Cr II The analysis of this spectrum was completed in all wavelength regions by Sansonetti et al. [32, 33]. The spectra recorded for this work are among those currently being used for a comprehensive analysis of Cr I by both NIST and ICL.

Mn II The last extensive analysis of this spectrum was by Iglesias & Velasco [34]. A comprehensive analysis in all wavelength regions is currently being led by ICL, using both FT and grating spectra from NIST and ICL. Hyperfine structure parameters have been measured for 28 levels using fast ion-beam laser spectroscopy by Holt et al. [35]. Constants for an additional 47 levels were obtained by Townley-Smith et al. [23] using FT spectra from NIST and ICL .

Fe II The analysis of this spectrum has been completed in all wavelength regions by Nave & Johansson [21].

Co II This spectrum was measured using FT spectroscopy in the region 142 nm to 3300 nm by Pickering et al. [36–38]. Wavelengths for 145 lines below 142 nm were published by [39]. Comparison of Iglesias's energy levels with those of Pickering shows errors of up to 0.6 cm^{-1} , implying errors in Iglesias's wavelengths of 0.001 nm or more. We have recorded additional grating spectra in this wavelength region with the aim of reducing the wavelength uncertainty below 140 nm by an order of magnitude and identifying more lines using the levels in [36].

Ni II The most recent comprehensive analysis is that of Shenstone in 1970 [40] and covers the region 72.7 nm to 1000 nm. His analysis includes wavelengths below 222 nm that were measured on our normal incidence spectrograph, but he comments that *“the accuracy of the measurement throughout the whole spectrum is not as great as I had hoped”*. We have recorded new spectra using FT and grating spectroscopy to reduce the uncertainty of these wavelengths and are currently analyzing them to optimize the energy levels and extend the term analysis.

FIG. 5: Lines in the spectrum of an iron hollow-cathode lamp that correspond to features in the spectrum of χ Lupi. Black line is the observed spectrum taken from the data of Brandt et al. [42]. The red line is a synthetic spectrum based on the calculations of Kurucz[20], also taken from Brandt et al. The wavelength in nm of features in the laboratory spectrum of an iron-neon hollow cathode lamp are indicated above the plot. Only the line at 125.373 nm corresponds to a transition between two known energy levels in Fe II [21].

VI. EXTENSION OF SPECTRAL ANALYSIS USING STELLAR SPECTRA

The progress reported in the previous section represents a significant effort to complete the singly-ionized iron-group elements by both NIST and ICL. It is adding many thousands of lines to NIST Atomic Spectra Database [41], with improvements in the wavelength uncertainty of over an order of magnitude compared to the previous work. However, even this effort is insufficient to identify all lines of potential importance in stellar spectra. Fig. 5 shows a section of the spectrum of the chemically-peculiar star χ Lupi in the region around 125 nm observed with the Goddard High-Resolution Spectrograph on the Hubble Space Telescope [42]. Ten of the features in the stellar spectrum correspond to spectral lines in the laboratory spectrum of an iron hollow cathode lamp and are thus likely to be due to Fe II. Only one of these lines corresponds to a transition between known energy levels in Fe II.

In an effort to address this discrepancy between the laboratory data and the requirements of stellar spectroscopy, a number of researchers have been using the stellar spectra instead

of laboratory data in order to extend the term analysis. For this process to be reliable, it is important to compare stars of different temperatures, metallicities, and chemical abundances of the element in question. The possible existence of high-excitation lines of Fe II in the stars HR 6000 and HD 186122 was first noted in the proceedings of a previous ASOS meeting [43], and subsequently Castelli et al. used these stellar spectra to find new levels in Fe II [44, 45] and Mn II [1]. More recently, additional levels in Fe I were found by Peterson & Kurucz [46]. While there is always a danger of mis-identifying lines in these complicated stellar spectra, this approach offers a way of extending the analysis beyond what can be done using laboratory spectroscopy. Laboratory lists of unidentified lines then become important, as they would be able to confirm the species of a particular line in a stellar spectrum.

VII. CONCLUSIONS

The combination of FT spectroscopy with high-resolution grating spectroscopy has been a valuable tool for improving atomic spectroscopic data. The high quality of FT spectra enables accurate wavelengths to be determined that are valuable not only for determining astrophysical properties but also for extending the analysis of atomic spectra. High resolution grating spectroscopy enables weaker lines to be seen in the UV and VUV regions that are not detected using FT spectroscopy. The joint effort between NIST and ICL to improve the wavelengths and energy levels of singly-ionized iron-group elements has resulted in new analyses for iron, chromium, vanadium, and cobalt, with work on manganese, nickel, scandium and titanium in progress. Despite these intensive efforts, many spectral lines from iron-group elements are likely to remain unidentified in stellar spectra and new approaches will be needed in the future.

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