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Measurement and calculation of L-shell transitions in M-shell iron ions

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Abstract
We have made high-resolution measurements of the iron L-shell emission near 15 Å using the EBIT-I electron beam ion trap at Livermore that exhibit L-shell transitions from autoionizing levels in Fe^{13+}, Fe^{14+} and Fe^{15+} ions. The observed L-shell iron spectra were modeled using the flexible atomic code augmented with transition energies produced by calculations based on the relativistic multi-reference Møller–Plesset (MRMP) perturbation theory, allowing us to identify multiple M-shell iron lines. Our measured values for the Fe XV emission lines are in excellent agreement with a recent measurement using the BESSY-II synchrotron but the present measurements have somewhat higher accuracy. Our MRMP calculations are compared to earlier calculations using the many-body perturbation theory approach, and we find good agreement for some but not all transitions.

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(Some figures may appear in color only in the online journal)

1. Introduction

L-shell x-ray transitions from M-shell iron ions, i.e. transitions connecting electrons in the L shell with levels in the $n \geqslant 3$ shell in iron ions with more than ten electrons, have become of great interest to x-ray astronomy after it has been discovered that they contribute to absorption features in the iron L-shell spectrum near 15 Å [1, 2]. These lines are difficult to calculate accurately because the upper levels involve core excitation with M-shell spectator electrons and, thus, are subject to strong electron–electron correlation effects.

Gu *et al* [2] have used the many-body perturbation theory (MBPT) approach to predict the L-shell transition energies of M-shell iron ions. Here, we present results from calculations based on the relativistic multi-reference Møller–Plesset (MRMP) perturbation theory [3, 4], which agree with the MBPT calculations in most but not all cases.

L-shell transitions in M-shell iron ions are difficult to observe spectroscopically from collisional sources because the excitation energy (about 800 eV) greatly exceeds the energy for ionization of the respective parent ion (100–500 eV), which means that few ions exist in the desired charge state. Moreover, the excited levels have a high autoionization rate, which further reduces the photon yield. Measurements were recently made at BESSY-II, which exploited the high autoionization rate of these levels [5]. The BESSY-II experiments used a novel combination of target ions from an electron beam ion trap and an energetic sychrotron beam that excited L-shell electrons in Fe^{14+} ions to the $n = 3$ levels and recorded the production of Fe^{15+} ions by the subsequent Auger decay via particle counting methods. As the energy of synchrotron beam was scanned over these photo-ionization resonances, precise determination of various energy levels in Fe^{14+} ions could be made.

Employing the EBIT-I electron beam ion trap we searched for L-shell transitions of M-shell iron ions in emission beyond those from Fe^{15+} that we reported earlier [6]. This search was successful, and we were able to observe many new emission features. The energies we determined for Fe^{14+} transitions are in good agreement with those measured in the BESSY-II experiments, but they are somewhat more accurate.

Table 1. Comparison of our MRMP results with earlier MBPT results. All transitions are to the ground level.

Ion	Upper level	MBPT [2] (Å)	MRMP (Å)
Fe^{15+}	$2p_{1/2}2p^4_{3/2}3s_{1/2}3d_{5/2}$ $(J = 3/2)$	15.265	15.266
	$2p_{1/2}2p^4_{3/2}3s_{1/2}3d_{3/2}$ $(J = 1/2)$	15.209	15.211
	$2p_{1/2}2p^4_{3/2}3s_{1/2}3d_{3/2}$ $(J = 3/2)$	15.113	15.111
Fe^{14+}	$2s^2_{1/2}2p_{1/2}2p^4_{3/2}3s^2_{1/2}3d_{5/2}$ $(J = 1)$	15.358	15.358
	$2s^2_{1/2}2p^2_{1/2}2p^3_{3/2}3s^2_{1/2}3d_{5/2}$ $(J = 1)$	15.597	15.592
	$2s_{1/2}2p^2_{1/2}2p^4_{3/2}3s^2_{1/2}3d_{5/2}$ $(J = 1)$	14.183	14.179
Fe^{13+}	$2p_{1/2}2p^4_{3/2}3s^2_{1/2}3p_{1/2}3d_{3/2}$ $(J = 3/2)$	15.634	15.638
	$2p_{1/2}2p^4_{3/2}3s^2_{1/2}3p_{1/2}3d_{3/2}$ $(J = 1/2)$	15.556	15.573
	$2p_{1/2}2p^4_{3/2}3s^2_{1/2}3p_{3/2}3d_{3/2}$ $(J = 3/2)$	15.610	15.614

2. Calculations

Our calculations were carried out using the MRMP approach described by Ishikawa [3, 4]. Results from such calculations have been reported earlier for L-shell transition of Fe^{15+} ions [7], and more details of these calculations are presented in [8]. Results of our MRMP calculations for the three lines in Fe^{13+}, Fe^{14+} and Fe^{15+} ions, for which MBPT calculations have been reported by Gu *et al* [2], are shown in table 1.

Inspecting table 1, we find that there are no (measurable) differences between our calculations and those of Gu *et al* for Fe^{15+}. For the Fe^{14+} transitions we find very good agreement with the MBPT results of Gu *et al* for all three transitions. By contrast, two out of the three Fe^{13+} transitions agree within 4 mÅ. However, the third transition differs by 17 mÅ. Measurements are clearly needed to decide which calculation produces the more accurate results.

We also carried out calculations with the flexible atomic code (FAC) [9] in order to model the measured spectral intensities. The calculations included electron-impact excitation, radiative cascades and autoionization. We combined these FAC calculations with the MRMP results to have reliable estimates of the line positions.

3. Experiment

The measurements were carried out on the EBIT-I electron beam ion trap at Livermore [10]. Spectra were recorded at beam energies of 1500 and 2000 eV, in order to maximize the counting efficiency by being able to operate the electron beam at a higher current than otherwise possible. Because M-shell iron ions ionize away very quickly at such high energies, we have used a 3 ms measurement cycle, after which the ions were dumped. The methodology is thus similar to the measurements of the K-shell iron emission performed earlier [11–13]. Those measurements were made using a metal vapor vacuum arc injector, which provides pulsed injection of iron. Here, we injected iron in a continuous stream in the form of iron pentacarbonly using the EBIT-I gas injection system. The injection pressure was kept high (10^{-6} Torr), in order to maximize the radiation from M-shell iron ions. In this regard, the measurement is very similar to our earlier measurement of the K-shell spectrum from L-shell oxygen ions [14, 15].

We used a high-resolution grating spectrometer to record the iron L-shell emission near 15 Å [16]. A typical spectrum

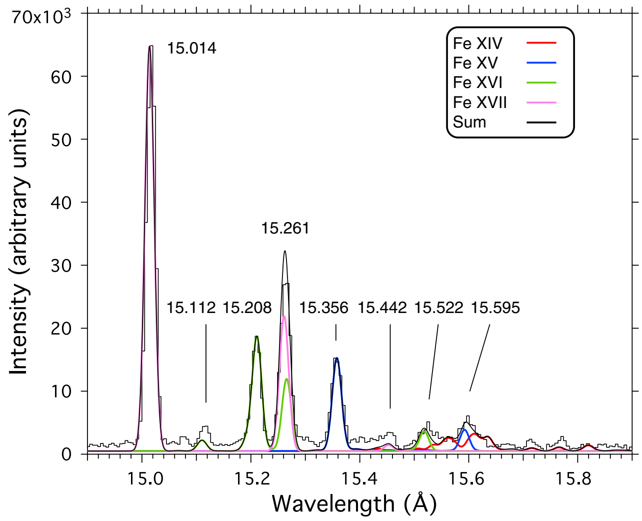

Figure 1. L-shell emission spectrum of iron near 15 Å. The spectrum is fitted using FAC intensity predictions for Fe XIV (red trace), Fe XV (blue trace), Fe XVI (green trace) and Fe XVII (pink trace) modified with the wavelengths from the MRMP calculations. The measured position of each line (in Å) is indicated in the figure.

obtained at a beam energy of 1500 eV is shown in figure 1. Unfortunately, the high beam energy means that charge states higher than Fe^{16+} can be produced. Indeed, we see evidence of Fe XVIII emission in the spectra; the Fe XVIII (and higher) L-shell emission was reported earlier [17, 18].

The wavelength scale was calibrated by measuring well known reference lines from heliumlike neon and hydrogenlike oxygen in separate spectra. Lines from hydrogenlike and heliumlike oxygen can also be seen in the iron spectra, and their lines provide an anchor to fix the wavelength calibration.

The measured spectra were compared to our modeling calculations, as illustrated in figure 1. This comparison enabled us to identify the two strongest 3d → 2p Fe XV lines, as indicated in the figure. The modeling calculations also indicate the presence of Fe XIV lines. However, unlike the two Fe XV features, all Fe XIV features are blends, and no individual Fe XIV lines could yet be identified.

4. Comparison of the Fe^{14+} results with theory and BESSY-II results

The results of our Fe XV measurements are given in table 2. They agree well with our MRMP calculations and the earlier MBPT calculations of Gu *et al* [2]. They also agree well with the results from BESSY-II reported by Simon *et al* [5]. They do not agree with the very recent Breit–Pauli *R*-matrix (BPRM) calculation by Hasoglu *et al* [19]. These employed a semi-empirical energy shift based on the NIST ionization and excitation energy values. Hasoglu *et al* pointed out that the NIST values appear incorrect, and the comparison in table 2 supports this notion.

Table 2. Comparison of measured Fe XV level energy values from EBIT-I and BESSY-II with theory. The uncertainty of each measurement is given in parentheses.

Upper level	MBPT [2]	MRMP (this work)	BPRM + NIST [19]	BESSY-II [5]	EBIT-I (this work)
$2s_{1/2}^2 2p_{1/2} 2p_{3/2}^4 3s_{1/2}^2 3d_{5/2}$ $(J = 1)$	794.95	795.16	798.77	794.70(20)	794.95(10)
$2s_{1/2}^2 2p_{1/2}^2 2p_{3/2}^3 3s_{1/2}^2 3d_{5/2}$ $(J = 1)$	807.25	807.30	811.13	807.10(20)	807.29(05)

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