

Article

Measurement and Flexible Atomic Code (FAC) Computation of Extreme Ultraviolet (EUV) Spectra of Eu

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Abstract: A group of EUV lines of H- and He-like ions of C provides excellent wavelength calibrations for a position-sensitive multichannel detector at a high-resolution spectrograph. We have exploited this setting for a series of spectra of highly charged Eu ions recorded at the Livermore SuperEBIT electron beam ion trap. A variation in the electron beam energy results in spectra with correspondingly staggered highest Eu ion charge states ranging from Na- through to Ni-like Eu ions. A number of spectral features can be identified from the literature, but the majority of line identifications need guidance from computations of simulated spectra on the basis of collisional-radiative models. For ions with more than two electrons in the valence shell, the typical computational results are of a markedly lower accuracy. We have applied the Flexible Atomic Code (FAC), which is capable of handling all our measured ions with reasonable accuracy. We look into the systematics of the deviation of the computed transition energies from the measured ones as a function of the electron number.

Keywords: atomic spectra; highly charged ions; extreme ultraviolet (EUV); electron beam ion trap; flexible atomic code FAC



Citation: Clementson, J.H.T.; Beiersdorfer, P.; Brown, G.V.; Hell, N.; Träbert, E. Measurement and Flexible Atomic Code (FAC) Computation of Extreme Ultraviolet (EUV) Spectra of Eu. *Atoms* **2024**, *12*, 48. <https://doi.org/10.3390/atoms1210048>

Academic Editor: John Sheil

Received: 27 August 2024

Revised: 20 September 2024

Accepted: 24 September 2024

Published: 27 September 2024



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1. Introduction

The extreme ultraviolet (EUV) spectra of highly charged ions of rare earth elements are of interest both on their own and for the problem of analyzing the somewhat similar W spectra of future fusion reactors. Most accurate wavelength data are wanted. We have taken advantage of a group of EUV lines of H- and He-like ions of C (C VI, C V) that provide excellent wavelength calibrations for our high-resolution spectra recorded at the Livermore SuperEBIT electron beam ion trap. A variation in the electron beam energy permits the production of spectra with a systematically varied highest ion charge state contributing. Thus, many lines can be associated with specific charge state ions, and all the spectra (of Na- through Ni-like Eu ions) are calibrated against the same reference data [1–3]. To help with the line identifications, computations are needed for simulating spectra on the basis of collisional-radiative models. Such simulations reveal the general structure of the individual spectra, as well as the approximate wavelength values. For the spectra of ions with only one or two electrons in the valence shell (in our data, Na- and Mg-like ions), extensive computations compete with the experiment for accuracy (see [1]). For ions with more than two electrons in the valence shell, the typical computational results are of a markedly lower accuracy. We have applied the Flexible Atomic Code (FAC) [4], which is capable of handling all our measured ions with moderate effort and reaches reasonable accuracy. However, the complexity of the computational problem increases with the number of electrons in the atomic system. We therefore look into the systematics of the deviation of the computed transition energies from the measured ones as a function of the electron number.

2. Experiment

The Livermore SuperEBIT electron beam ion trap [5–7] was fed by a directed vapour stream of heated Eu atoms [8], all under ultrahigh vacuum conditions. A tightly collimated

electron beam of adjustable energy in the range 2.2 keV to 38 keV crossed the atom cloud and collisionally excited and ionized atoms. The freshly produced ions experienced the electric and magnetic fields of the trap arrangement and thus were confined, so that subsequent collisions of fast electrons with ions could result in further stepwise ionization until the ionization potential of the ions exceeded the available collision energy. Although fresh atoms were continually supplied and then ionized through all intermediate charge states, the charge balance in the stored ion cloud comprised mostly ions near the maximum achievable charge states under the given conditions. The series of experiments employed various spectrometers and detectors for the extreme ultraviolet (EUV) [1–3] and X-ray (XR) ranges [9–13], of which we discuss only the EUV data here. The series of measurements at a variety of electron beam energy settings are expected to yield the spectra of the ions of the isoelectronic sequences from Na (11 electrons) to Zn (30 electrons).

Two high-resolution grazing-incidence grating spectrographs (HiGGS) [14] with variable line spacing gratings of Rowland circle radius $R = 44.3$ m and 2400 L/mm groove spacing, and equipped with position-sensitive CCD detectors, observed the same trapped ion cloud in EUV light, as did the ECS microcalorimeter [15] in the X-ray range. In the EUV, near the resonance lines of C V (≈ 40 Å) and C VI (≈ 34 Å), the 25 mm wide CCD chip covers a wavelength interval of about 10 Å width that comprises the C VI 1s-2p Ly_α line and the C V 1s²-1snp resonance line series up to $n = 6$, and thus excellent wavelength references with much better than 1 mÅ reliability. This accuracy amounts to roughly 30 ppm. A slightly parabolic fit curve establishes the wavelength scale for the measured spectra. The intensity of the carbon lines in the spectra can be regulated by the admission of CO₂ (at ultrahigh vacuum-compatible density) that also serves as a coolant for the highly charged ions in the trap (see [1]). The small shifts in the detector position extend the working range to an interval of about 12 Å that can be anchored to the same reference lines. The wavelengths of isolated and statistically viable Eu lines can be measured in these spectra with accuracies higher than 100 ppm, irrespective of the ion charge state. However, only for Na- and Mg-like ions, there are computations, the results of which agree with the measured wavelength at this level, see the examples and discussion in [1].

3. Computation

Accurate computations of atomic structure at the 100 ppm level are very demanding and have not been routinely achieved for ions with more than two electrons in the valence shell, not even by the same experts applying the same techniques that have been successful for one-, two-, three-, eleven- or twelve-electron ions. The increase in the scatter of predictions when adding a single electron to the valence shell has been remarkable. In the framework of our study of Eu spectra we have turned to a practical, though less accurate, approach instead: we used the Flexible Atomic Code (FAC) developed by Gu [4]. This code can run on a laptop or on a multiprocessor supercomputer, and accordingly it can be set to various numerical atomic structure computational approaches and to different expected levels of accuracy. We used a laptop version and the option of Relativistic Configuration Interaction (RCI) computations.

For each of the Eu ions from Na-like to Zn-like, we used configuration state functions that permitted the valence electron to occupy the valence shell or any level up to $n = 5$ or 6 (the latter for the iron group element—like ions). An additional electron excitation was permitted from the 2*l* or 3*l* level in the highest shell below the ground state valence electron. All radiative transitions were computed, and the most prominent collisional excitations (from low-lying levels), as well as autoionisation. Of the millions of computed spectral lines, only those that exceeded an intensity of 3% in the strongest line of a given ion in the EUV range were considered for the evaluation.

Our FAC computations were intended to provide orientation in our attempt of interpreting a set of spectra on which hardly any literature data were available. They were not intended to serve as a database for future reference. Any full-scale atomic structure computational exercise with that intention would exceed the present effort by more than an

order of magnitude. For that reason it seems moot to record all the settings of the program as used in our exploratory run.

A comparison of our measured EUV spectra of Eu with the output of our FAC computations supports about 30 line identifications of relatively prominent spectral features (see [3]). Closer scrutiny might yield as many additional classifications of less prominent lines, but those identifications ought to be augmented by preceding further data accumulation which is expected to yield a more statistically significant signal.

4. Discussion

Figure 1 shows the relative difference of the computed and measured term differences for most of the presently identified Eu lines in our spectra on a scale using parts per thousand (per mille). All the predicted wavelengths are shorter than the measured ones; that is, all term differences are computed as higher than observed. This is a typical finding in most atomic structure computations. It can be argued that this finding relates to the Ritz principle, according to which the lowest level of a given symmetry is always computed higher than the true value, because any error in the wave function should lead to such a trend.

Figure 1 also indicates that the deviation increases roughly linearly with the number of electrons (see the eye-guiding line). The data display begins with the Na-like ions; here, the FAC results differ from the experiment by roughly 1300 ppm (1.3 per mille). For the Mg-like ion, the difference is twice as large, indicating that the present FAC results are more than an order of magnitude less accurate than the extensive state-of-the-art computations performed and discussed by Santana et al. [16]. However, that publication demonstrates that many of the published atomic structure computations of Mg-like ions perform considerably less well. The difference between FAC results and measurement increase further along the sequence of ions with increasing electron numbers. For ions that are isoelectronic with iron group elements, the deviation reaches 6 to 8 per mille. This is quite competitive with the typical results of several established atomic structure theory packages. In the displayed range of ions, several shell closures occur. These are reflected in the relative minima along the general trend.

A striking outlier is the single data point for the Ti-like ion (with a deviation of the FAC result from the experiment of about 14 per mille), which has similarly been reported in the literature spectra of other elements. There is a known peculiarity in the $3p^6 3d^4$ ground configuration of Ti-like ions; the $J = 2 - 3$ interval is almost constant for a wide range of atomic numbers [17] and has proven challenging to atomic structure calculations (see [18] and the references therein). It is possible that the difficult theoretical treatment of this configuration is responsible for the larger than average deviation of the computed transition energy from observation.

Equally striking is the high intensity of the signature line of the Ti-like ion spectrum [2,3], which is apparently a $3p^6 3d^4 J = 0 - 3p^5 3d^5 J = 1$ transition. A signal rate markedly higher than all other lines in the neighbouring ion charge states and this wavelength band suggests that a funneling effect may be involved in the population of the upper level that captures the decays of several other levels. However, the decay chain that feeds this level has not yet been investigated for such a peculiarity. Interestingly, an experiment on dielectronic recombination at one of the Shanghai electron beam ion traps has detected the presence of a particularly long-lived level in Ti-like ions of W [19].

There are several other Ti-like ion transitions predicted in our wavelength band, but the predicted line intensities are lower by more than an order of magnitude. These lines have not yet been identified.

Figure 1 reveals that four lines in the V-like Eu ion have been identified with practically the same offset of the FAC results from measurement, and similar groups may be found in the Mn- and Fe-like ions. In contrast, the Cr-like ion offers four candidates for line identification, but with a considerable spread of the predictions compared to the experimental data.

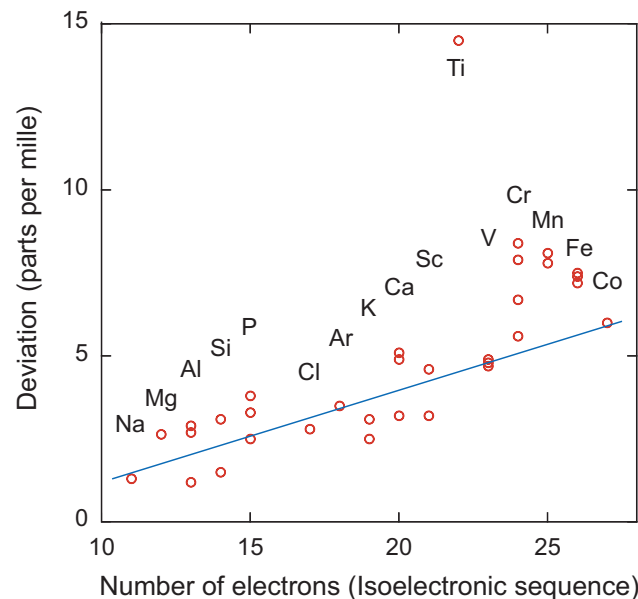


Figure 1. The relative deviation (red circles) of the computed transition energies (by FAC) from the measured ones in Eu ions with 11 to 27 electrons. The blue eye-guiding line suggests a roughly linear trend up to $Z = 27$ (Co), and more pronounced deviations from the trend for elements near Fe.

Author Contributions: Experiment, E.T., N.H. and G.V.B.; methodology, P.B.; computation, J.H.T.C.; data analysis and curation, E.T.; resources, P.B.; writing—original draft preparation, E.T.; writing—review and editing, all authors; funding acquisition, P.B. All authors have read and agreed to the published version of the manuscript.

Funding: This research received no external funding.

Data Availability Statement: The original contributions presented in the study are included in [3]. Further inquiries can be directed to the corresponding author.

Acknowledgments: This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract No. DE-AC52-07NA27344.

Conflicts of Interest: The authors declare no conflicts of interest.

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