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Abstract. Spectroscopic measurements on few-electron high-Z ions take guidance from isoelectronic trends of low-Z to mid-Z ions and from theory. Such wide-range extrapolations, however, are fraught with uncertainty. We discuss as examples some n=3, Δn=0 transitions in the EUV spectra of Na-, Mg- and Al-like ions of Au that have been observed by electron beam ion trap work and by heavy-ion accelerator based beam-foil spectroscopy. New insights are gained from notable recent progress of calculations.

1. Introduction

The spectra of highly charged ions feature interesting properties because relativistic contributions dominate atomic structure, and quantum electrodynamical corrections become notable. Only two techniques so far have reached ionization stages as high as Na-, Mg- or Al-like Au (Z=79) ($Au^{68+,67+,66+}$). One of these is beam-foil spectroscopy [1, 2, 3], the other employs an electron beam ion trap (EBIT) [4]. In the first technique, the fast ions interact mostly with the practically free electrons in a target at rest. In the second, a beam of fast electrons interacts with trapped target ions practically at rest.

Beam-foil spectroscopy at high ion energies encounters various physics problems that do not beset EBIT. Among these is the Doppler shift that needs to be determined precisely if reliable wavelength data are to be extracted. Next, the ion-foil interaction can lead to multiple excitation, with the result of line-rich spectra that may be difficult to analyze. A unique advantage of the beam-foil light source lies in its inherent time resolution. Recent calculations have indicated possible problems with the interpretation of the aforementioned beam-foil data on Au. It seemed worthwhile to try an EBIT observation of the same transitions.

2. EBIT experiment

Our work was done at Livermore (LLNL), using the EBIT-II electron beam ion trap [5]. Au ions from a metal vapor vacuum arc ion source (MeVVA) were further ionized by multiple collisions with the fast electrons of the high-current density electron beam. Electron beam energies from 3 keV (for comparison with our earlier data [4]) up to 17.5 keV (the maximum energy attainable with one stage of the high-voltage power supply damaged) were employed to reach maximum ion charge states up to Na-like Au^{67+}. This is about twice the threshold energy for the production of the desired charge states $Au^{66+,67+,68+}$. The beam current ranged from 80 mA at the lower energies to 150 mA at the higher ones. The ions were kept inside the trap for about 10 s; then the trap was purged in order to prevent the accumulation of unwanted heavy contaminants.

The light from the trapped ion cloud was observed by a flat-field spectrometer [6] equipped with a variable-line spacing grating (radius of curvature R=15 m) having a 2400 ℓ/mm central line density and a cryogenic thinned, back-illuminated charge-coupled device (CCD) multichannel detector. The available CCD camera system had a higher dark rate than the better one owned by the group (both manufactured by Photometrics, Inc.), which was tied up in another experiment. The detector has 1024 × 1024 pixels of 25 μm pixel size. Along the spectrum, about 900 channels were evaluated, while across the dispersion direction the spectra - after filtering for cosmic ray spot events - were binned in order to improve the signal-to-noise ratio. The spectrometer arrangement worked without an extra entrance slit, imaging instead the 70-μm diameter excitation zone directly onto the detector. This source size corresponds to a minimum line width of about three pixels.

The thermal background distribution on the CCD chip was measured by recording spectra while inverting the trap voltages (drift tube voltages), thus expelling any multiply charged ions from the trap volume. There also were found patterns in the read-out noise. Both noise sources contribute to the background spectra. In order to avoid doubling the effective noise, smooth functions averaging the background were used instead of raw background data. A typical exposure of 20 minutes was sufficient to produce the n=4 - n'=4 lines of Ge- to Cu-like ions of Au as observed previously. Exposures at various electron beam energies showed how these charge states burn out at electron beam energies beyond about 8 keV. However, none of the n=3 - n'=3 transitions of present interest could be recognized in individual spectra recorded at 10 to 17.5 keV. Only after summing a total of 63 spectra (21 h total accumulation time) recorded at 15 and 17.5 keV, respectively, could spectral features be discerned (Fig. 1).

The full spectra covered the range from about 2.6 to 9.8 nm in a single setting. They were calibrated with the well known 1s - 2p transitions in H-like ions of C and in He-like ions of C (3.3736/4.0268 nm) and N (2.8787 nm), prominent 4-4 transitions in Ge- to Cu-like Au [4] (observed at lower electron beam energies), and a number of lines from Li-like ions of Ne [7]. The Ne spectra were recorded in separate observations. The calibration curve permitted wavelength determinations to better than 0.005 nm. However, we resorted to this value as a conservative estimate. Our EBIT-II wavelength results are given in Table 1.

3. Results and discussion

In the preceding heavy-ion accelerator beam-foil experiments on Au [1, 2, 3], the EUV spectra at ion-beam energies near 13 MeV/amu showed lines and partially resolved line clusters that comprised the 3s-3p$_{1/2}$ resonance transition in Na-like Au^{68+}, the 3s^2 $^1S_0$ - 3s3p $^3P^o_1$ intercombination transition in Mg-like Au^{67+}, the 3s^{2}3p $^2P^o_{3/2}$ - 3s3p^2 $^4P_{5/2}$ transition in Au^{66+}, the much weaker 3s^{2}3p $^2P^o_{1/2}$ - 3s3p^2 $^4P_{1/2}$ transition in the same ion, and a number of weak lines. The linewidths were 0.13 Å [2] and 0.085 nm [3], respectively. The EBIT spectrum in Fig. 1 in contrast shows only three clearly recognizable lines in the range of interest, with line widths of 0.03 nm. The initial line identification followed the beam-foil study, but the line positions and

relative intensities seemed somewhat odd. In view of the inconsistencies and several contradictive predictions, the data remained unpublished.

None of the weak lines seen in the beam-foil spectra appeared in the EBIT spectra, possibly a sign of the very different excitation processes in the two devices. In the low density electron beam ion trap the environment the collisionally excited ions regularly have time to decay radiatively before they are excited again. Consequently only those levels can be expected to be populated that are reached by direct excitation from the ground state. This observation provides one clue to the line identities of Fig. 1. The other clue is from the notable progress in better algorithms for atomic structure calculations. A recent addition to the atomic structure calculation arsenal is the Multi-Reference Møller-Plesset algorithm and procedure [8, 9, 10], which has been remarkably successful in a number of cases, describing many-electron systems with a precision that rivals the available spectroscopic data. When applied to the present case of highly charged Au ions, the MR-MP results for Na-like ions come very close to the proven reference calculations by Kim *et al.* [15] and thus also to the measured wavelength of one of our three EUV lines of interest. For the other two, the calculations indicate identifications that are different from the previous educated guesses. According to the new calculations, the long wavelength line (instead of the short wavelength one) is to be identified with the intercombination transition in the Mg-like ion, and the short wavelength line instead coincides with the wavelength prediction for the $3s^2 3p\ ^2P^o_{1/2}$ - $3s3p^2\ ^4P_{1/2}$ transition in the Al-like ion (Table 1). The $3s^2 3p\ ^2P^o_{3/2}$ - $3s3p^2\ ^4P_{5/2}$ line of the Al-like ion, the dominant line in some of the beam-foil spectra, is gone; it results from multiple (high-density) excitation, whereas the EBIT light source provides a low density environment. None of the other lines discussed in the beam-foil work would be expected to be prominent under this constraint - and none is seen.

4. Conclusion

Even with a rather small spectrometer on ENBIT-II, meaningful wavelength data have been obtained on ions as highly charged as q=66+ to 68+. The experimental wavelengths in turn provide feedback on the quality of recent calculations. A fruitful interplay of experiment and theory is now becoming possible. Details of how this applies to a reanalysis of the beam-foil data on Xe and Au are being presented elsewhere [11, 12].

5. Acknowledgments

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Table 1. Wavelength values (nm) for the Au^{q+} $3s^k3p^l$ - $3s^{k-1}3p^{l+1}$ transitions studied in this work.

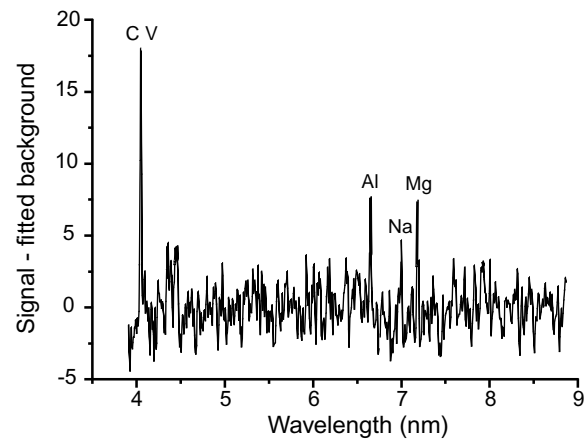| Experiment	Ref.	Theory	Ref.
Au^{66+} $3s^23p$ $^2P^o_{1/2}$ - $3s3p^2$ $^4P_{1/2}$			
6.60±0.02	[3]	6.525	[13]
6.643±0.005	This work	6.646	This work
Au^{68+} $3s$ $^2S_{1/2}$ - $3p$ $^2P^o_{1/2}$			
		6.9973	[14]
		6.997	[15]
6.993±0.005	This work	7.001	This work
Au^{67+} $3s^2$ $^1S_0$ - $3s3p$ $^3P^o_1$			
		6.80	[16] (interpolated)
		7.263	[17]
		7.172	[18]
7.182±0.005	This work	7.185	This work

Figure 1. Sum of 63 spectra of Au, recorded at electron beam energies of 15 keV and 17.5 keV, respectively, after background subtraction. Na, Mg, and Al denote the isoelectronic sequences of the Au lines identified in Table 1.