UCRL-JRNL-223518

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August 8, 2006

Journal of Physics

Relativistic atomic data for EUV and X-ray spectra of highly charged Cu-, Zn-, Ga- and Ge-like ions ($70 \leq Z \leq 92$)

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Abstract. Wavelengths and transition probabilities have been calculated for the n=4, Δn=0 allowed transitions in the heavy Cu-, Zn-, Ga- and Ge-like ions with Z=70-92. Fully relativistic multiconfiguration Dirac-Fock (MCDF) computations were carried out. The present results are compared to and agree well with recent electron-beam ion-trap (EBIT) measurements in Yb, W, Os, Au, Pb, Bi, Th and U ions.

1. Introduction

Recently, accurate experimental wavelengths for high Z ($Z \geq 70$) elements were measured at the Livermore electron beam ion trap (EBIT) for some transitions in the EUV and X-ray spectra of highly charged ytterbium ($Z = 70$), tungsten ($Z = 74$), osmium ($Z = 76$), gold ($Z = 79$), lead ($Z = 82$), bismuth ($Z = 83$), thorium ($Z = 90$) and uranium ($Z = 92$) along the copper, zinc, gallium and germanium isoelectronic sequences [1-8]. In these latter works, it was pointed out that available calculations for these ions, carried out with different theoretical approaches, featured different isoelectronic trends (relative to the experimental trend). These new measurements justify a detailed theoretical analysis of radiative parameters for heavy ions ($Z \geq 70$) along the isoelectronic sequences. The new theoretical results will be useful as a test of experimental observations, and their predictive power will be valuable where experimental data are missing.

2. Theoretical method

In the present work, energy levels, wavelengths and transition rates for the $n = 4$, $\Delta n = 0$ transitions in highly charged Cu-, Zn-, Ga- and Ge-like ions were obtained using the fully relativistic multiconfiguration Dirac-Fock (MCDF) approach with the latest version of GRASP, the General-purpose Relativistic Atomic Structure Package, developed by Norrington [9] from the original MCDF code of Grant and coworkers [10-11] and improved by Dyall *et al* [12]. The computations were done with the extended average level (EAL) option, optimizing a weighted trace of the Hamiltonian using level weights proportional to $2J+1$. The orthogonality of the wavefunctions was consistently included in the differential equations by using off-diagonal Lagrange multipliers. Most of the configurations belonging to the n=4 complex were included in the calculations. These configurations are listed in the following subsections. They are expected to take the most important configuration interaction effects into account for the high ionization stages considered in the present work. The calculations were then completed with the inclusion of the relativistic two-body Breit interaction and of the the quantum electrodynamic corrections (QED) due to self-energy and vacuum polarization using the routines developed by McKenzie *et al* [11]. In these routines, the leading correction to the Coulomb repulsion between electrons in quantum electrodynamics is considered as a first perturbation using the transverse Breit operator given by Grant and McKenzie [13], the second order vacuum polarization corrections are evaluated using the prescription of Fullerton and Rinker [14], and the self-energy contributions are estimated by interpolating the hydrogenic n=1,2 results of Mohr [15-16] and by scaling to higher n states according to $1/n^3$. For each ion, the nuclear effects were estimated by considering a uniform charge distribution in the nucleus with the usual atomic weight.

2.1. Cu-like ions from Yb^{41+} to U^{63+}

The wavelengths and transition rates for the 4s-4p, 4p-4d and 4d-4f transitions were obtained using the following non-relativistic configurations in the calculations: $3d^{10}4s$, $3d^{10}4d$, $3d^94s^2$, $3d^94s4d$, $3d^94p^2$, $3d^94p4f$, $3d^94d^2$, $3d^94f^2$, $3d^84s^24d$, $3p^53d^{10}4s4p$, $3p^53d^{10}4s4f$, $3p^53d^{10}4p4d$, $3p^53d^{10}4d4f$, $3s3p^63d^{10}4s^2$, $3s3p^63d^{10}4s4d$, $3s3p^63d^{10}4p^2$, $3s3p^63d^{10}4p4f$, $3s3p^63d^{10}4d^2$, $3s3p^63d^{10}4f^2$ (even parity) and $3d^{10}4p$, $3d^{10}4f$, $3d^94s4p$, $3d^94s4f$, $3d^94p4d$, $3d^94d4f$, $3d^84s^24p$, $3d^84s^24f$, $3p^53d^{10}4s^2$, $3p^53d^{10}4s4d$, $3p^53d^{10}4p^2$, $3p^53d^{10}4p4f$, $3p^53d^{10}4d^2$, $3p^53d^{10}4f^2$, $3s3p^63d^{10}4s4p$, $3s3p^63d^{10}4s4f$, $3s3p^63d^{10}4p4d$, $3s3p^63d^{10}4d4f$ (odd parity). This corresponds to 1494 relativistic configuration state functions.

2.2. Zn-like ions from Yb^{40+} to U^{62+}

For these ions, results were obtained for the $4s^2$–4s4p, 4s4p–$4p^2$ and 4s4p–4s4d transitions. All of the even and odd configurations belonging to the n=4 complex were included in the calculations. These configurations were $4s^2$, $4p^2$, $4d^2$, $4f^2$, 4s4d, 4p4f and 4s4p, 4s4f, 4p4d, 4d4f for each parity, respectively, and were expected to take the most important configuration interaction effects into account for the high ionization stages considered.

2.3. Ga-like ions from Yb^{39+} to U^{61+}

The wavelengths and transition probabilities for the $4s^24p$–$4s^24d$ and $4s^24p$–$4s4p^2$ transitions were obtained using, in the MCDF calculations, all of the odd configurations except $4p4f^2$ and $4f^3$ and all of the even configurations except $4s4f^2$ and $4d4f^2$ within the n=4 complex. These configurations are $4s^24p$, $4s^24f$, 4s4p4d, 4s4d4f, $4p^3$, $4p^24f$, $4p4d^2$, $4d^24f$ and $4s^24d$, $4s4p^2$, 4s4p4f, $4s4d^2$, $4p^24d$, 4p4d4f, $4d^3$ for the odd and even parities, respectively, and generate a total of 437 relativistic configuration state functions (CSFs).

2.4. Ge-like ions from Yb^{38+} to U^{60+}

The following non-relativistic configurations were considered in the calculations: $4s^24p^2$, $4s^24p4f$, $4s^24d^2$, $4s^24f^2$, $4s4p^24d$, 4s4p4d4f, $4p^4$, $4p^24d^2$, $4p^24f^2$ (even parity) and $4s^24p4d$, $4s^24d4f$, $4s4p^3$, $4s4p^24f$, $4s4p4d^2$, $4s4p4f^2$, $4s4d^24f$, $4p^34d$, $4p^24d4f$, $4p4d^3$ (odd parity). This corresponds to 1526 relativistic configuration state functions.

3. Results

A large amount of radiative parameters (wavelengths and transition rates) were obtained along the copper, zinc, gallium and germanium isoelectronic sequences. The complete sets of data will be published elsewhere [17-20]. In Table 1, we report a sample of results showing a comparison between the MCDF wavelengths and those measured in EBIT devices [1-8] and in laser-produced plasmas [21-24] for the 4s J=1/2 – 4p J'=3/2 and the 4s^2 J=0 – 4s4p J'=1 resonance transitions in Cu-like and Zn-like ions, respectively.

Table 1. Comparison between MCDF wavelengths obtained in the present work and those measured experimentally for resonance transitions in Cu- and Zn-like ions.

Seq.	Transition	Z	Ion	MCDF	Experiment	
				This work	EBIT	Other
Cu	4s J=1/2 – 4p J'=3/2	70	Yb XLII	76.014	75.8595(47)[3]	75.842(15)[23]
		74	W XLVI	62.444	62.3355(45)[3]	
					62.3355(19)[2]	62.304(15)[22]
		76	Os XLVIII	56.652	56.5630(20)[5,7]	
		79	Au LI	49.006	48.9280(26)[3]	48.928(15)[21]
					48.92(1)[1]	
		82	Pb LIV	42.441	42.3740(58)[3]	42.349(15)[21]
		83	Bi LV	40.463	40.4066(20)[5,7]	40.394(15)[21]
		90	Th LXII	29.054	29.0227(10)[5,7]	28.990(15)[21]
					29.0224(30)[3]	
		92	U LXIV	26.452	26.4233(15)[5,7]	26.400(15)[21]
					26.4325(19)[3]	26.406(15)[23]
Zn	4s^2 J=0 – 4s4p J'=1	70	Yb XLI	73.464	73.8070(66)[4]	73.792(20)[24]
		74	W XLV	60.676	60.9300(54)[4]	60.900(20)[24]
					60.9310(17)[2]	
		76	Os XLVII	55.178	55.3840(50)[8]	
		79	Au L	47.883	48.0583(49)[4]	48.063(20)[24]
					48.05(1)[1]	
		82	Pb LIII	41.584	41.7185(45)[4]	41.689(20)[24]
		83	Bi LIV	39.680	39.8151(20)[8]	39.792(20)[24]
		90	Th LXI	28.639	28.7227(67)[4]	28.702(20)[24]
					28.7303(11)[8]	
		92	U LXIII	26.106	26.1868(36)[4]	26.157(20)[24]
					26.1861(10)[8]	

In Figures 1 and 2, we show the wavelength differences between our MCDF calculations and the experimental measurements for some resonance transitions in the different sequences. It can be observed that the differences between EBIT measurements and MCDF calculations show a smooth behaviour along the sequences, $\Delta\lambda$ decreasing monotically with increasing Z while striking discontinuities can be noticed when comparing calculated wavelengths with those measured in laser-produced plasmas for Cu-like and Zn-like ions. This can be explained by the fact that, contrary to laser-produced plasma experiments, EBIT devices are able to select charge states and therefore to avoid blends between lines of different charge states that can deteriorate the accuracy of the wavelength measurements. Another explanation, as suggested by Kim *et al.* [25], would be the alteration of the line profiles by self-absorption in high density plasmas produced by laser.

4. Acknowledgements

PQ, PP and EB are respectively Research Associates and Research Director of the Belgian FNRS. ET thanks the German Research Association (DFG) and the US Department of Energy

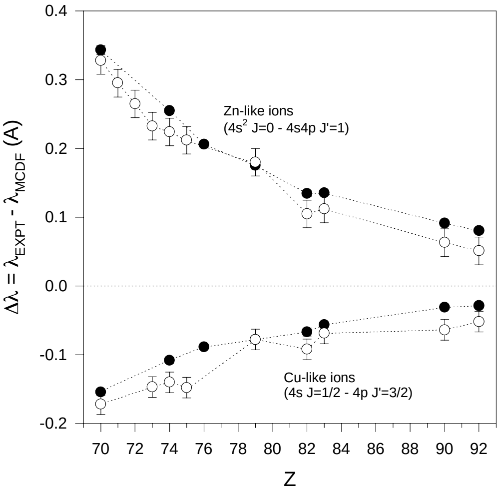

Figure 1. Comparison between experimental and MCDF wavelengths for transitions in Cu- and Zn-like ions. Full and open symbols correspond to EBIT and laser-produced plasma experiments, respectively.

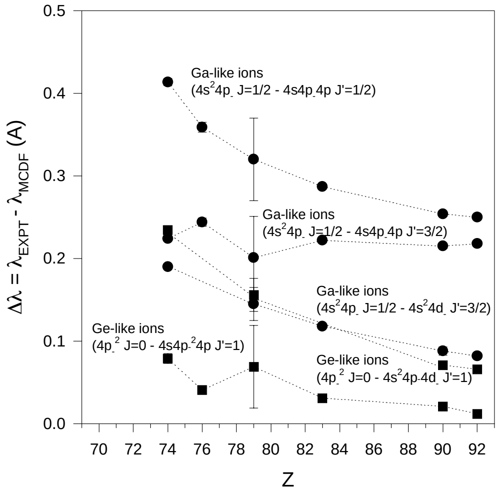

Figure 2. Comparison between experimental and MCDF wavelengths for transitions along the Ga (circles) and Ge (squares) isolectronic sequences.

by University of California Lawrence Livermore National Laboratory (Contract W-7405-Eng-48).

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