

Discrepancies between calculated and observed energies for $4s\text{-}4p$ transitions in highly charged Cu-like ions

J. F. Seely and U. Feldman

E. O. Hulburt Center for Space Research, Naval Research Laboratory, Washington, D.C. 20375-5000

A. W. Wouters, J. L. Schwob,* and S. Suckewer

Princeton Plasma Physics Laboratory, Princeton University, Princeton, New Jersey 08544

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The $4s_{1/2}\text{-}4p_{1/2}$ and $4s_{1/2}\text{-}4p_{3/2}$ transitions in the Cu-like ions of the elements Sn, Xe, La, Nd, Eu, Gd, Dy, and Yb (atomic numbers $Z = 50, 54, 57, 60, 63, 64, 66,$ and 70) have been observed in the spectra from the Princeton Large Torus tokamak. The experimentally determined transition energies were compared to the transition energies calculated using the multiconfiguration Dirac-Fock technique. By including previously published observations, the experimental and calculated transition energies were compared for the entire Cu I isoelectronic sequence from Ru ($Z = 44$) to U ($Z = 92$). Contrary to the conclusion of Cheng and Wagner [Phys. Rev. A **36**, 5435 (1987)], we find significant discrepancies between the experimental and calculated transition energies. The discrepancies are attributable to electron correlation corrections that are not accounted for in the calculation.

I. INTRODUCTION

Transitions in highly charged ions of the elements Au, Pb, Bi, Th, and U were observed by Seely *et al.*¹ in the spectra from laser-produced plasmas. The transition energies for the Cu-like $4s_{1/2}\text{-}4p_{1/2}$ and $4s_{1/2}\text{-}4p_{3/2}$ transitions were calculated using the multiconfiguration Dirac-Fock (MCDF) computer package developed by Grant *et al.*,^{2,3} and it was demonstrated¹ that the measured wavelengths were sufficiently accurate for the determination of the QED contributions to the transition energies. Cheng and Wagner⁴ recalculated the transition energies including finite nuclear size effects, and they concluded that there were no significant differences between the calculated and experimental transition energies for the Cu-like $4s_{1/2}\text{-}4p_{1/2}$ and $4s_{1/2}\text{-}4p_{3/2}$ transitions. Cheng and Wagner⁴ included in their comparisons all of the available experimental data for the elements from Sn to U (atomic number $Z = 50\text{--}92$).

In this paper we present new wavelength measurements for the Cu-like $4s_{1/2}\text{-}4p_{1/2}$ and $4s_{1/2}\text{-}4p_{3/2}$ transitions in the elements Sn, Xe, La, Nd, Eu, Gd, Dy, and Yb. This work greatly expands the number of observations for the $4s_{1/2}\text{-}4p_{1/2}$ transition that are available for comparison with the calculations. The experimental transition energies were compared to the transition energies calculated using the MCDF techniques of Cheng and Wagner.⁴ We find significant discrepancies between the experimental and calculated transition energies. Since the Grant MCDF program is widely used to calculate transition energies, it is important to resolve the differences between the experimental and calculated transition energies.

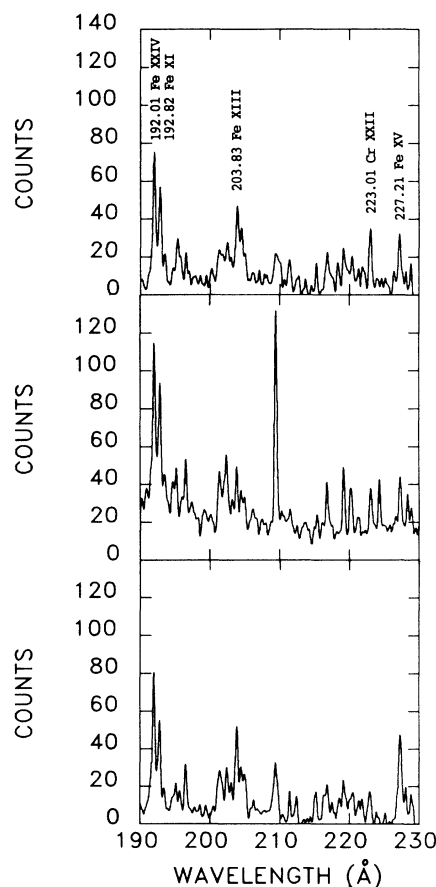


FIG. 1. Time sequence of PLT spectral scans in the wavelength region 190–230 Å recorded every 100 msec. The injection of La occurred at the time of spectrum (b), and the line at 209.40 Å is the $4s_{1/2}\text{-}4p_{1/2}$ transition in La^{28+} .

II. EXPERIMENT

The spectra were generated by injecting the elements of interest into the Princeton Large Torus (PLT). The electron temperature of the Ohmically heated discharge (approximately 2 keV) was raised to 4.5–6.0 keV by adding radio-frequency power at the lower hybrid frequency for a period of 200 msec. The element of interest was injected 50 msec after the start of the rf pulse. The elements Sn, La, Nd, Eu, Gd, Dy, and Yb were injected using the laser blow-off technique. Xe was injected using the gas-puff technique. The electron density at the time of injection was approximately $2 \times 10^{13} \text{ cm}^{-3}$.

The spectra were recorded by a 2-m grazing-incidence spectrometer that was described in Ref. 5. The spectrometer was fitted with a 600 groove/mm grating, and spectra were recorded from approximately 50 to 340 Å. The spectra were detected by a flat MgF_2 -coated microchannel plate that was coupled to a 1024-pixel photodiode array by a fiber-optic transmission line. During each discharge, a wavelength region that was approximately 50-Å wide was recorded. Spectral scans were recorded every 100 msec throughout the discharge. The details of the data reduction techniques were described in Refs. 6–8.

A time sequence of spectral scans is shown in Fig. 1 for the case of La injection. Before the time of injection, the spectra were composed of transitions in highly charged ions of the elements from the wall material (C, O, Cr, Fe, and Ni). At the time of injection, strong spectral features from the injected element appeared superimposed on the background spectrum. The transitions in the injected element were intense in one or two scans in the time sequence of scans, and the transitions in the injected element were easily distinguished from the relatively steady background transitions. The Cu-like $4s_{1/2}-4p_{1/2}$ and $4s_{1/2}-4p_{3/2}$ transitions were typically among the most intense transitions in the injected element.

As discussed in Ref. 7, the wavelength scale was estab-

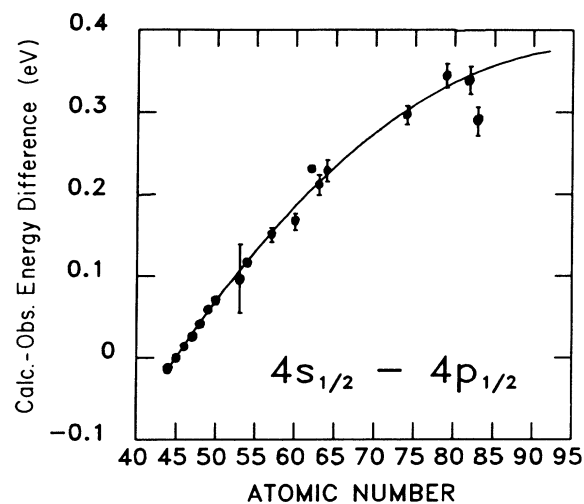


FIG. 2. Comparison of the calculated and observed $4s_{1/2}-4p_{1/2}$ transition energies. The observed transition energies are from Table II, and the error bars represent the uncertainties in the observed transition energies. The curve is a least-squares fit to the differences between the calculated and observed transition energies.

lished using a large number of transitions in the background elements as references. Wavelength corrections were made to account for the nonlinearities in the fiber-optic taper and in the pixel positions. The uncertainty in the wavelength scale was estimated to be ± 0.01 Å. The spectral lines were typically 0.3-Å wide which corresponded to six pixels. The uncertainty in the measured wavelengths of the transitions in the injected elements is estimated to be ± 0.03 Å.

The identification of the Cu-like $4s_{1/2}-4p_{1/2}$ and $4s_{1/2}-$

TABLE I. Observed wavelengths (in Å) for the $4s_{1/2}-4p_{3/2}$ and $4s_{1/2}-4p_{1/2}$ transitions.

Z	Ion	$4s_{1/2}-4p_{3/2}$			$4s_{1/2}-4p_{1/2}$		
		Observed Present	Observed Previous	Calculated Present	Observed Present	Observed Previous	Calculated Present
50	Sn^{21+}	219.00	218.978 ^a	219.067	276.11	276.065 ^a	275.681
54	Xe^{25+}	173.93	173.938 ^b	173.915	233.98	233.959 ^b	233.448
57	La^{28+}	147.54	147.565 ^c	147.558	209.40		208.870
60	Nd^{31+}	125.92	125.896 ^c	125.852	189.04		188.562
63	Eu^{34+}	107.82	107.829 ^d	107.757	171.98	171.3 ^e	171.478
64	Gd^{35+}	102.43	102.459 ^d	102.395	166.88		166.369
66	Dy^{37+}	92.61	92.652 ^e	92.538			156.889
70	Yb^{41+}	75.85	75.816 ^d	75.800		140.9 ^e	140.429

^aReader, Acquista, and Cooper (Ref. 9).

^bKaufman, Sugar, and Rowan (Ref. 10).

^cReader and Luther (Ref. 11).

^dDoschek *et al.* (Ref. 12).

^eFinkenthal *et al.* (Ref. 14).

TABLE II. The observed (λ_o), calculated (λ_c), and fitted (λ_f) wavelengths (in Å) for the $4s_{1/2}-4p_{1/2}$ transition for Ru^{15+} - U^{63+} . The uncertainty in the observed wavelength is $\Delta\lambda_o$.

Z	λ_o	$\Delta\lambda_o$	λ_c	$\lambda_c - \lambda_o$	λ_f	$\lambda_f - \lambda_o$
44	374.286 ^a	0.010	374.416	0.130	374.267	-0.019
45	353.564 ^a	0.010	353.565	0.001	353.577	0.013
46	334.975 ^a	0.010	334.838	-0.137	334.977	0.002
47	318.130 ^a	0.010	317.917	-0.213	318.156	0.026
48	302.871 ^a	0.010	302.551	-0.320	302.868	-0.003
49	288.943 ^a	0.010	288.530	-0.413	288.908	-0.035
50	276.11 ^b	0.030	275.681	-0.429	276.107	-0.003
51			263.861		264.323	
52			252.949		253.439	
53	243.3 ^c	0.200	242.839	-0.461	243.349	0.049
54	233.959 ^d	0.005	233.448	-0.511	233.972	0.013
55			224.697		225.231	
56			216.524		217.063	
57	209.40 ^b	0.030	208.870	-0.530	209.411	0.011
58			201.686		202.227	
59			194.928		195.466	
60	189.04 ^b	0.030	188.562	-0.478	189.095	0.055
61			182.549		183.076	
62	177.45 ^e	0.010	176.865	-0.585	177.384	-0.066
63	171.98 ^b	0.030	171.478	-0.502	171.989	0.009
64	166.88 ^b	0.030	166.369	-0.511	166.871	-0.009
65			161.511		162.003	
66			156.889		157.371	
67			152.485		152.956	
68			148.282		148.742	
69			144.267		144.716	
70			140.429		140.866	
71			136.753		137.179	
72			133.231		133.646	
73			129.851		130.254	
74	126.99 ^f	0.015	126.606	-0.384	126.998	0.008
75			123.487		123.868	
76			120.489		120.858	
77			117.600		117.958	
78			114.818		115.165	
79	112.485 ^g	0.015	112.135	-0.350	112.472	-0.013
80			109.549		109.875	
81			107.052		107.368	
82	104.94 ^g	0.015	104.640	-0.300	104.946	0.006
83	102.55 ^g	0.015	102.306	-0.244	102.602	0.052
84			100.047		100.333	
85			97.861		98.137	
86			95.770		96.037	
87			93.723		93.981	
88			91.745		91.994	
89			89.824		90.064	
90			87.973		88.205	
91			86.163		86.387	
92			84.431		84.647	

^aReader, Acquista, and Cooper (Ref. 9).

^bPresent work.

^cJohnson *et al.* (Ref. 13).

^dKaufman, Sugar, and Rowan (Ref. 10).

^eFinkenthal *et al.* (Ref. 14).

^fSeely *et al.* (Ref. 15).

^gSeely *et al.* (Ref. 1).

$4p_{3/2}$ transitions was based on the time dependence of the spectral features, the calculated wavelengths, and the previous observations where available. The wavelengths were calculated using the MCDF computer package developed by Grant *et al.*^{2,3} and using the same techniques as Cheng and Wagner.⁴ The calculations included QED, Breit, and finite nuclear size effects. The optimal level (OL) option of Grant's program was used, and the calculations therefore included one configuration. The observed and calculated wavelengths are listed in Table I.

All of the presently observed $4s_{1/2}$ - $4p_{3/2}$ transitions have been previously observed in high-resolution spectra from laser-produced plasmas or the Texas Experimental Tokamak⁹⁻¹² (TEXT). The presently measured wavelengths for the $4s_{1/2}$ - $4p_{3/2}$ transition agree with the previous high-resolution measurements to within ± 0.04 Å. The $4s_{1/2}$ - $4p_{1/2}$ transition was previously observed for Sn (Ref. 9) and Xe (Ref. 10) in high-resolution spectra and for Eu and Yb (Ref. 14) in low-resolution spectra (± 0.7 Å).

Listed in Table II are the calculated wavelengths and the best available observations from the present work and previous^{1,9,10,13-15} work for the Cu-like $4s_{1/2}$ - $4p_{1/2}$ transition in the elements Ru¹⁵⁺ through U⁶³⁺ ($Z=44-92$). The calculated and observed transition energies are compared in Fig. 2, where the error bars represent the uncertainties in the observations. The calculated transition energies differ significantly from the observations, and the differences tend to increase with Z .

The observed wavelengths were semiempirically corrected by fitting a polynomial in Z to the differences between the calculated and observed $4s_{1/2}$ - $4p_{1/2}$ transition energies. The least-squares fit is shown by the curve

in Fig. 2. The resulting fitted wavelengths are listed in Table II, and the deviations of the fitted wavelengths from the observed wavelengths are given in the last column in Table II. In a similar manner, the $4s_{1/2}$ - $4p_{3/2}$ wavelengths were semiempirically corrected by fitting the differences between the calculated and observed wavelengths to a polynomial.¹⁶

III. TRANSITION ENERGIES

The calculated $4s_{1/2}$ - $4p_{1/2}$, $4s_{1/2}$ - $4p_{3/2}$, and $4p_{1/2}$ - $4p_{3/2}$ energy intervals for five representative ions are listed in Table III. These calculated energies are compared to the energies derived from the fitted wavelengths for the $4s_{1/2}$ - $4p_{1/2}$ and $4s_{1/2}$ - $4p_{3/2}$ transitions. The differences between the calculated and fitted energies are given by the last column in Table III. Significant differences occur for all of the intervals and ions listed in Table III. The calculated $4s_{1/2}$ - $4p_{1/2}$ energies are consistently too large, and the calculated $4p_{1/2}$ - $4p_{3/2}$ energies are consistently too small by a comparable amount. The calculated $4s_{1/2}$ - $4p_{3/2}$ energies are in better agreement with the fitted values.

It is clear from Fig. 2 and Table III that the differences between the calculated and observed energies greatly exceed the estimated experimental uncertainties. This implies that the differences between the calculated and observed energies are experimentally significant. This conclusion differs from the findings of Cheng and Wagner.⁴ Although Cheng and Wagner⁴ found differences between the calculated and observed energies that were comparable to the differences derived in the present work, Cheng and Wagner⁴ concluded that the

TABLE III. The calculated and fitted energies (in eV). For each ion, the first row is $4s_{1/2}$ - $4p_{1/2}$, the second row is $4p_{1/2}$ - $4p_{3/2}$, and the third row is $4s_{1/2}$ - $4p_{3/2}$. FNS stands for finite nuclear size, VP for vacuum polarization, and SE for self-energy corrections.

Z	Ion	Coulomb ^a	FNS ^b	Breit	VP	Corrections ^c		Fitted ^e	Fitted-calc. difference ^f
						SE	Total ^d		
54	Xe ²⁵⁺	53.121	-0.022	0.250	0.049	-0.288	53.110	52.991 $\pm$ 0.002	-0.119 $\pm$ 0.002
		18.414	0.000	-0.258	0.002	0.023	18.180	18.290 $\pm$ 0.004	0.110 $\pm$ 0.004
		71.535	-0.022	-0.008	0.051	-0.265	71.290	71.281 $\pm$ 0.004	-0.009 $\pm$ 0.004
64	Gd ³⁵⁺	74.600	-0.086	0.560	0.127	-0.677	74.524	74.300 $\pm$ 0.004	-0.224 $\pm$ 0.004
		47.092	-0.003	-0.594	0.008	0.058	46.560	46.720 $\pm$ 0.013	0.160 $\pm$ 0.013
		121.692	-0.089	-0.034	0.135	-0.620	121.084	121.020 $\pm$ 0.012	-0.064 $\pm$ 0.012
74	W ⁴⁵⁺	98.236	-0.297	1.067	0.286	-1.362	97.929	97.628 $\pm$ 0.008	-0.301 $\pm$ 0.008
		102.216	-0.019	-1.202	0.028	0.115	101.140	101.350 $\pm$ 0.033	0.210 $\pm$ 0.033
		200.452	-0.316	-0.135	0.314	-1.247	199.069	198.978 $\pm$ 0.032	-0.091 $\pm$ 0.032
79	Au ⁵⁰⁺	111.134	-0.540	1.416	0.416	-1.859	110.568	110.237 $\pm$ 0.010	-0.331 $\pm$ 0.010
		144.534	-0.042	-1.658	0.050	0.152	143.036	143.276 $\pm$ 0.053	0.240 $\pm$ 0.053
		255.668	-0.582	-0.241	0.466	-1.708	253.604	253.512 $\pm$ 0.052	-0.092 $\pm$ 0.052
92	U ⁶³⁺	149.451	-2.500	2.736	1.032	-3.871	146.848	146.473 $\pm$ 0.02	-0.375 $\pm$ 0.02
		326.329	-0.318	-3.603	0.209	0.234	322.851	323.150 $\pm$ 0.18	0.299 $\pm$ 0.18
		475.780	-2.818	-0.867	1.241	-3.636	469.700	469.623 $\pm$ 0.18	-0.077 $\pm$ 0.18

^aThe Coulomb energy for a point nucleus.

^bThe finite nuclear size (FNS) correction to the Coulomb energy.

^cThe Breit, vacuum polarization (VP), and self-energy (SE) corrections including finite nuclear size contributions.

^dThe total calculated energy.

^eThe energy derived from the semi-empirically corrected wavelengths for the $4s_{1/2}$ - $4p_{1/2}$ and $4s_{1/2}$ - $4p_{3/2}$ transitions. The estimated uncertainty in the fitted wavelengths is ± 0.010 Å, and the corresponding uncertainty in the energy is indicated.

^fThe difference between the fitted and calculated energies.

TABLE IV. The calculated second- and third-order Coulomb correlation corrections E_{corr} and the discrepancies with observations (in eV). For each ion, the first row is $ns_{1/2}-np_{1/2}$, the second row is $np_{1/2}-np_{3/2}$, and the third row is $ns_{1/2}-np_{3/2}$.

Z	Ion	$n=2^a$	E_{corr}	$n=3^b$	Discrepancies $n=4^c$
54	Xe^{25+}	-0.258		-0.240	-0.119 ± 0.002
		0.113		0.091	0.110 ± 0.004
		-0.145		-0.149	-0.009 ± 0.004
74	W^{45+}	-0.361		-0.296	-0.301 ± 0.008
		0.254		0.204	0.210 ± 0.033
		-0.107		-0.093	-0.091 ± 0.032
92	U^{63+}	-0.544		-0.368	-0.375 ± 0.02
		0.502		0.390	0.299 ± 0.18
		-0.042		0.022	-0.077 ± 0.18

^aReference 18.

^bReference 19.

^cTable III.

differences were not significant.

The differences between the calculated and observed energy intervals may, in general, result from inaccuracies in the calculated energies, inaccuracies in the observed energies, or a combination of both. Owing to the extent and consistency of the observations (see Fig. 2 and Table II), it is most likely that the differences between the calculated and observed energies result primarily from inaccuracies in the calculation.

Inaccuracies in the energies that are calculated using Grant's program may arise in the correction terms (self-energy, vacuum polarization, Breit, and finite nuclear size). In addition, electron correlation corrections to the Coulomb and Breit energies are not included in Grant's program and may also be significant.

The QED corrections (self-energy and vacuum polarization) that are calculated by Grant's program are derived from the hydrogenic values and a screened nuclear charge.³ It is often asserted that these calculated QED corrections are rather inaccurate. While this may be true for multielectron ions with complex configurations, it has been shown that the calculated QED corrections for the Li-like $2s_{1/2}-2p_{1/2}$ and $2s_{1/2}-2p_{3/2}$ transitions are quite accurate,¹⁷ and it can be shown that the same is true for the Na-like $3s_{1/2}-3p_{1/2}$ and $3s_{1/2}-3p_{3/2}$ transitions. It is likely that the calculated QED corrections for the Cu-like $4s_{1/2}-4p_{1/2}$ and $4s_{1/2}-4p_{3/2}$ transitions are also rather accurate. As shown in Table III, the differences between the calculated and observed $4p_{1/2}-4p_{3/2}$ energies are comparable to or larger than the calculated QED corrections, and possible errors in the QED calculation cannot account for the large $4p_{1/2}-4p_{3/2}$ discrepancies. Similarly, the $4p_{1/2}-4p_{3/2}$ discrepancies are comparable to or larger than the calculated finite nuclear size corrections. We conclude that possible errors in the calculated QED and finite nuclear size corrections cannot account for the large $4p_{1/2}-4p_{3/2}$ discrepancies.

The Breit correction is large for both the $4s_{1/2}-4p_{1/2}$ and $4p_{1/2}-4p_{3/2}$ intervals and is smaller for the $4s_{1/2}-4p_{3/2}$ interval. However, the calculated Breit corrections should be quite accurate. The Breit corrections for the Li-like $2s-2p$ and Na-like $3s-3p$ transitions that are calcu-

lated using Grant's program are in excellent agreement with the many-body perturbation theory calculations of Johnson *et al.*^{18,19}

It is often assumed that the Coulomb correlation correction is nearly independent of Z .⁴ This is true for the lowest-order correction to the nonrelativistic energy.²⁰ However, when using a Dirac-Fock basis, relativistic effects cause the Coulomb correlation correction to vary with Z . In Ref. 18 and 19, the second- and third-order Coulomb correlation corrections were calculated for the $ns_{1/2}-np_{1/2}$ and $np_{1/2}-np_{3/2}$ (where $n=2,3$) intervals in Li-like and Na-like ions. It was found that the absolute values of the $ns_{1/2}-np_{1/2}$ and $np_{1/2}-np_{3/2}$ corrections increase with Z , and the $ns_{1/2}-np_{3/2}$ corrections decrease with Z . The Coulomb correlation corrections for $Z=54, 74$, and 92 are shown in Table IV. The trend in these corrections for $n=2$ and $n=3$ is consistent with the observed discrepancies for $n=4$ (from Table III). The correlation corrections to the Breit term may be comparable to the correlation correction to the Coulomb term and may also contribute to the discrepancies.

IV. CONCLUSION

New observations for the Cu-like $4s_{1/2}-4p_{1/2}$ and $4s_{1/2}-4p_{3/2}$ transitions have been combined with previously published results and compared with the transition energies calculated using Grant's program. Significant discrepancies between the observed and calculated transition energies occur. While inaccuracies in the calculation of the correction terms (self-energy, vacuum polarization, finite nuclear size, and Breit) may contribute to the discrepancies, the discrepancies are believed to result primarily from the omission in the Grant program of correlation corrections to the Coulomb (and possibly Breit) terms.

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*Permanent address: Racah Institute, Hebrew University of Jerusalem, 91904 Jerusalem, Israel.

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