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New spectroscopic data for atomic tungsten XIV

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Abstract. The thirteen times ionized tungsten is isoelectronic with PmI. Wavelengths and transition probabilities for the 5s-5p and 5p-5d transitions of WXIV, identifying the ground state as $4f^{13}\ 5s^2\ ^2F_{7/2}$ were calculated**.** Both, a relativistic Hartree Fock approach, including core-polarization effects, and a purely relativistic multiconfiguration Dirac-Fock method were used for the calculations. Particularly, 5s-5p transitions were compared with experimental results obtained with VUV electron beam ion trap (EBIT) spectroscopy.

1. Introduction

The thirteen times ionized tungsten (WXIV) is isoelectronic with PmI. Reliable spectroscopic parameters in the tungsten atom are of fundamental importance for the study of fusion plasmas, but some discrepancies remain unsolved. On one hand, Curtis and Ellis [1], using a nonrelativistic single-configuration model, identified the collapse of the 4f orbital and predicted the wavelengths for 5s-5p transitions setting the ground state as [Kr] $4d^{10}\ 4f^{14}\ 5s\ ^2S_{1/2}$. On the other, Theodosiou and V. Raftopoulos [2] used a more sophisticated multiconfigurational relativistic approach to identify the ground state as $4f^{13}\ 5s^2\ ^2F_{5/2}$, but predicting the wavelengths of 5s-5p transitions far away from the experimental values [3].
In this work we made HFR[4] and GRASP [5] calculations for wavelength and transition probabilities for the 5s-5p (table 1) and 5p-5d (table 2) transitions, identifying the ground state as $4f^{13}\ 5s^2\ ^2F_{7/2}$ in accordance with the paper of Kramida [6], showing good agreement with the observed values of the reference [3]. We also took into account the core polarization effects that refer to the deformation of the internal atomic orbitals due to the orbit of the active electron, which repels the remaining electrons (section 2.2)

2. Theory and discussions

Three calculation methods were used in this paper to obtain the wavelengths gA and gf. For the first two methods, Cowan's package [4] was used, and the third method used the GRASP relativistic program [5].

2.1. The Relativistic Hartree–Fock method

In Cowan's package, wavefunctions are calculated in a Hartree–Fock approximation with relativistic corrections. The wavefunctions are used to calculate a multiconfigurational energy matrix. Both the eigenvalues and the eigenvectors of the matrix are functions of the Slater parameters, i.e., functions of the average configuration energy E_{ave}, electrostatic direct F^k and exchange G^k integrals,configuration

interaction integrals R^k, and spin–orbit parameters ζ_{nl}, as well as the coefficients of the multiconfigurational expansion (Ref. [4, Eq. (16.7)]). This method was used in several previous paper (see for example M.Raineri et.al Ref [7])
In this calculation the following configurations were included: $4f^{14}5s$, $4f^{14}5d$, $4f^{13}5s5p$, $4f^{13}5p5d$, $4f^{14}5p$, $4f^{13}5s^2$, $4f^{12}5s^25p$, $4f^{13}5p^2$ and $4f^{13}5s5d$ for both parities.
Figure 1 shows the average energy values (E_{ave}) along the promethium isoelectronic sequence of all configurations considered in our Relativistic Hartree-Fock calculation.

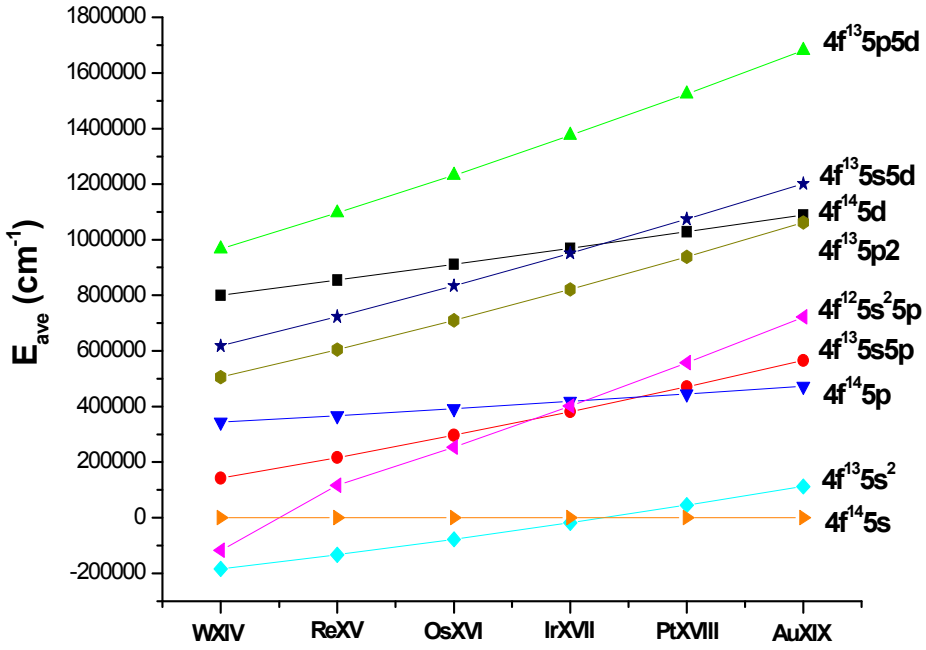

Figure 1. The average energy values (E_{ave}) along the promethium isoelectronic sequence of all configurations considered in our Relativistic Hartree-Fock calculation

In figure 1 we can observe that the ground state of Pm-like ions starting with W XIV, is the odd-parity $4f^{13}5s^2$ and in our relativistic approach it predicts the change to happen at Ir XVII. In accordance with the paper of Kramida [6] our HFR[4] and GRASP[5] calculations identify the ground state as $4f^{13}\ 5s^2\ ^2F_{7/2}$ separated from the first excited state $4f^{13}\ 5s^2\ ^2F_{5/2}$ by approximately 18000 cm^{-1}.

2.2 Hartree–Fock plus core polarization
We included the Core Polarization (CP) effects (see, for example, Curtis L.J. [8] and Biémont [9]) just by replacing the dipole integral

$$\int_0^\infty P_{nl}(r) r P_{n'l'}(r) dr \quad \rightarrow \quad \int_0^\infty P_{nl}\, r \cdot \left[1 - \frac{\alpha_d}{(r^2+r_c^2)^{3/2}}\right] P_{n'l'}(r) dr - \frac{\alpha_d}{r_c^3} \int_0^\infty P_{nl}(r) P_{n'l'}(r) dr$$

Here α_d is the electric dipole polarizability of the core, and r_c is the cut-off radius, which defines the boundaries of the atomic core. This is the same modification used by Quinet [10] to correct transition matrix elements when including CP effects. In our case, the radial functions were obtained from the

single configuration Hartree-Fock Method with relativistic corrections, and no modification was done to include CP effects in the Hamiltonian. As suggested by Migdalek & Baylis [11], core polarization approximately describes the core-valence correlation effects. As it is shown in table 1 and table 2 we present calculations with two values of the polarizability using different ion cores: one when the core has a $[Kr]4d^{10}5s^2$ (WXXVII) ($\alpha = 0.233 a_0^3$ [12] structure, and another for transitions that preserve the $[Kr]4d^{10}$ (WXXIX) core ($\alpha = 0.0716\ a_0^3$). For this last value of polarizability we considered the expression [4]:

$$\alpha_d = 4Ry^2 \sum_{yJ}^{M} f_{y'J',yJ}\ \lambda^2_{y'J',yJ}$$

where f is the oscillator strength of the transition, λ its corresponding wavelength, and Ry is the Rydberg constant.

2.3 Relativistic Dirac–Fock calculations

The GRASP package solves the Dirac equations within the framework of relativistic quantum theory [5]. This program offers energy levels wavelength and dipole transition rates from a multiconfigurational, relativistic approach. The configurations included in the calculation were: $4f^{14}5s$, $4f^{14}5d$, $4f^{13}5s5p$, $4f^{14}5p$, $4f^{13}5s^2$, $4f^{13}5p^2$ and $4f^{13}5s5d$.

3. Results and conclusion

In table1 and table 2 we present the calculations described above for transitions 5s-5p, 5p-5d respectively. The Slater parameters (section 2.1) were scaled at 85% of their RHF values. In table 1 we compared our results with the Reference [3] showing good accordance between λ_{HFR} for $5s\ ^2S_{1/2}$ - $5p^2P_{1/2}$ to experimental wavelength.

Table 1 Wavelengths, transition rates and oscillator strengths for 5s – 5p transition of WXIV

Transition	λ_{HFR} [Å]	λ_{MCDF} [Å]	$\lambda_{Ref[3]}$ [Å]	Experimental Wavelength[3]	Log gf	gA	gA CP $\alpha = 0.0716\ a_0^3$	gA CP $\alpha = 0.233\ a_0^3$
$5s\ ^2S_{1/2}$-$5p^2P_{1/2}$	365.9	372.1	366.2	365.3	-0.288	$2.564\ 10^{10}$	$2.203\ 10^{10}$	$1.843\ 10^{10}$
$5s\ ^2S_{1/2}$-$5p^2P_{3/2}$	264.2	263.2	263.7	258.2	0.145	$1.332\ 10^{11}$	$1.141\ 10^{11}$	$9.571\ 10^{10}$

Table 2 Wavelengths, transition rates and oscillator strengths for 5p–5d transition of WXIV

Transition	λ_{HFR} [Å]	λ_{MCDF} [Å]	Log gf	gA	gA CP $\alpha = 0.0716\ a_0^3$	gA CP $\alpha = 0.233\ a_0^3$
$5p\ ^2P_{1/2}$-$5d\ ^2D_{3/2}$	194.1	192.8	0.322	$3.711\ 10^{11}$	$3.231\ 10^{11}$	$2.955\ 10^{11}$
$5p\ ^2P_{3/2}$-$5d\ ^2D_{3/2}$	243.9	243.5	-0.433	$4.131\ 10^{10}$	$3.655\ 10^{10}$	$3.284\ 10^{10}$
$5p\ ^2P_{3/2}$-$5d\ ^2D_{5/2}$	233.9	233.2	0.532	$4.151\ 10^{11}$	$3.680\ 10^{11}$	$3.3020\ 10^{11}$

The difference between the various calculations can be summarized as follows: GRASP took into account relativistic effects by means of a more complete approach than Cowan's package by the HFR method; HFR took into account correlation effects in a more complete way. Finally, in the HFR + CP, not only were correlation effects considered more deeply, but core polarization effects were taken into account in the gA calculations for the different values of polarizabilities.

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