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Spectra and oscillator strengths of d–d and d–p transitions for cobalt-like Cd^{21+} ion

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Abstract. We calculate the spectra and oscillator strengths for highly ionized cobalt-like Cd^{21+} ions $3p^63d^9$–$3p^53d^{10}$, $3p^63d^9$–$3p^63d^84p$ transitions by using multi-configuration self-consistent field method program together with fitting formula proposed by us. The calculations have a good agreement with observations.

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Key words: highly ionized, energy level, fitting formula

1 Introduction

The proposition of Soft-X-Ray laser theory, which laser work material is cobalt-like Au^{52+} was verified by TIAP instrument [1]. It renewed the interest of research for highly ionized cobalt-like ions. Ions of the cobalt isoelectronic sequence have the ground configuration $3p^63d^9$. At the beginning of the sequence the lowest configuration with odd parity is $3p^63d^84p$. However, from Rb^{10+} on, the $3p^53d^{10}$ configuration takes its place. The correction between $3p^63d^9/^2D$ and $3p^53d^{10}/^2P$ gives rise to configuration combination.

Experimentally, these configuration transitions of cobalt-like ions were first observed by Edlén for Rb, Sr, Y, Zr, Mo, Pd, Ag, Cd, In, and Sn, although no wavelengths were reported [2]. Edlén's observed wavelengths can be inferred from the wave numbers given in his monograph, which also gives values for Br and Sb [3]. Later, Alexander reported wavelengths for these transitions in Y, Zr, Nb, and Mo [4]. Two of these transitions were observed by Burkhalter *et al.* for Sn^{23+} in a laser-produced plasma [5] . Burkhalter *et al.* [6] reported new wavelength values for Mo^{15+}. The same transitions in Sr^{11+} were given by Acquista and Reader [7] and revised values for Sr^{11+}, Y^{12+}, Zr^{13+}, Nb^{14+}, and Mo^{15+} by Ryabtsev and Reader [8]. The $3p^63d^9$–$3p^53d^{10}$ transitions of Ba^{29+}, La^{30+}, Nd^{33+}, Sm^{35+}, Gd^{37+}, Dy^{39+}, Er^{41+}, and Yb^{43+}

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were reported by Reader [9]. New wavelengths for these transitions in Ag^{20+}, Cd^{21+}, In^{22+}, and Sn^{23+} were given by Kononov [10]. The magnetic-dipole transition between the levels of the $3p^6 3d^9\,/^2D$ ground term has been observed in three cobalt-like ions: the magnetic-dipole transitions of Zr^{13+} and Mo^{15+} were observed in the PLT tokamak by Suckewer [11]; that of Nb^{14+} was observed in an electron cyclotron resonance ion source by Prior [12]. Ekberg *et al.* [13] gave new measurements for $3p^6 3d^9$–$3p^5 3d^{10}$ transitions of the ions from Sr^{11+} to Au^{52+} in laser-produced plasmas.

In this paper, we have theoretically calculated the wavelengths and oscillator strengths for highly ionized cobalt-like Cd^{21+} ions $3p^6 3d^9$–$3p^5 3d^{10}$, $3p^6 3d^9$–$3p^p 3d^8 4p$ transitions using multi-configuration self-consistent field method [14] together with the fitting formula proposed by us. The calculations have a good agreement with observations.

2 Fitting formulas

Up to the present day, it is difficult to solve a HFR equation of polyelectron system accurately. However, our real purpose is calculating accurately the known energy levels of atoms and predicting the unknown those, which can be achieved by using multi-configuration self-consistent field method together with fitting formula. So it is important to find a better fitting formula. Because the difference values ΔE between experimental measuring values and theoretical calculated values of multi-configuration self-consistent field method change smoothly along the isoelectronic sequence, we can achieve the least square fitting and find the fitting formula between ΔE and Z_c. In 1987, Wyart proposed a fitting formula [15]

$$E_{\rm fit} = -98751.4 + 55078 \times Z_c + 5618.86 \times Z_c^2 + 7.6414 \times Z_c^3 + Z_c^4. \tag{1}$$

In 1991, Matsushima *et al.* proposed another fitting formula [16]

$$E_{\rm fit} = A + BZ_c + \frac{CZ_c^2}{10} + \frac{DZ_c^3}{100} + \frac{EZ_c^4}{1000} + \frac{FZ_c^5}{1000000}. \tag{2}$$

According to the quantum electrodynamics effect of high-Z ions proposed by Gould *et al.* [17], which can move the energy levels of the isoelectronic sequence, we find that the quantum electrodynamics effect of high-Z ions is not considered in the formulas (1) and (2). So we have proposed a better formula, in which the quantum electrodynamics effect of high-Z ions is included, and it is expressed as

$$\Delta E = A + BZ_c + CZ_c^2 + DZ_c^3 + EZ_c^4 + FZ_c^5 + GZ_c^6 + HZ_c^7 + \text{ higher order terms}, \tag{3}$$

where Z_c,Z_c^2,Z_c^3, and Z_c^4 constant term is used for eliminating high order relativistic effect, remnant correlation energy and radiative corrections; Z_c^5 is used for eliminating high order Breit effect as in the formula (1) and (2). Z_c^6, Z_c^7, and higher order terms is used for eliminating the quantum electrodynamics effect of high-Z ions, which is proposed by us. All of above-mentioned effects are not considered by the multi-configuration self-consistent field

method program (Cowan's HFR program pack). In this paper, all of these effects are added in calculation results through the fitting formula (3).

The reasonableness of the fitting formula (3) is expressed as following. Because the electric field of atomic nucleus is stronger than that of atomic electrons for highly ionized ions, the electronic orbit of highly ionized ions is similar as that of hydrogen-like ions. For the hydrogen -like ions, its radial wave function can be expressed as

$$P_{nl}(r)=-\left(\frac{Z(n-1-1)!}{n^2\big((n+1)!\big)^3}\right)^{1/2}\rho^{l+1}e^{-\rho/2}L_{n+1}^{2l+1}(\rho), \tag{4}$$

$$L_{n+1}^{2l+1}(\rho)=\big((n+1)!\big)\sum_{k=1}^{2n-l-1}\frac{(-\rho)^k}{(n-l-1-k)!\times(2l+1+k)}. \tag{5}$$

The energy between electrons and atomic nucleus is

$$E_{l-n}^{nl}=\left\langle nl\left|\frac{2Z}{r}\right|nl\right\rangle\propto Z^2. \tag{6}$$

The kinetic energy of electrons is

$$E_{kln}^{nl}=\big\langle nl\big|-\nabla^2\big|nl\big\rangle=\left\langle nl\left|-\frac{d^2}{dr^2}+\frac{l_i(l_i+1)}{r^2}\right|nl\right\rangle\propto Z^2. \tag{7}$$

The coulomb energy between electrons and electrons is

$$E_{C-C}^{nl,n'l'}=\left\langle nl,n'l'\left|\frac{2}{r_{1,2}}\right|nl,n'l'\right\rangle-\left\langle nl,n't'\left|\frac{2}{r_{1,2}}\right|n'l',nl\right\rangle\propto Z. \tag{8}$$

Considering relativistic effect, the energy change is

$$E_m^{nl}=\frac{a^2}{2}\int_0^\infty P_{nl}(r)\big(\epsilon_i-V(r)^i\big)^2P_{nl}(r)dr\propto Z^5. \tag{9}$$

Considering radiative corrections, the energy change is

$$E_{kln}^{nl}\propto(Z-S_1)^2, \qquad E_{e-N}^{nl}\propto Z(Z-S_2)^3, \tag{10}$$

$$E_{e-e}^{nl,n'l'}\propto(Z-S_3), \qquad E_{M.D}\propto(Z-S_4)^4. \tag{11}$$

Finally, considering the quantum electrodynamics effect of high-Z ions [17], the erengy change is

$$\begin{aligned}E_{QED}=&n^{-3}(2\pi)m_0c^2\Big(\big(A_{40}+A_{41}\ln\big)(Za)^{-2}\Big)(Za)^4+A_{50}(Za)^5\\&+\Big(\big(A_{60}+A_{61}\ln\big)(Za)^{-2}+A_{62}\ln^2(Za)^{-2}\Big)(Za)^6+A_{70}(Za)^7\\&+\text{ higher order terms }\propto Z^4,Z^5,Z^6,Z^7,\cdots.\end{aligned} \tag{12}$$

In the fitting formula (1) and (2), the Z_c,Z_c^2,Z_c^3,Z_c^4,Z_c^5 and constant term are included, but the Z_c^6,Z_c^7 and higher order terms are not included, in which the quantum electrodynamics effect of high-Z ions is not considered. In our fitting formula (3), the Z_c^6,Z_c^7 and higher order terms are included so that the quantum electrodynamics effect of high-Z ions is considered, in which we suppose that the energy changes of all configurations caused by higher order terms are same and it is similar to the processing method of references [15, 16].

3 Calculation procedures

The Cowan's HFR program pack is used for our calculation, in which relativistic effect and Breit effect are considered already. According to selection rules of transitions and considering configuration combination, we select even parity configurations as $3p^63d^9$,$3p^63d^84s$,$3p^63d^84d$,$3p^63d^85s$,$3p^53d^94p$,$3p^53d^94f$ and odd parity configurations as $3p^53d^{10}$,$3p^63d^84p$,$3p^63d^84f$,$3p^53d^94s$,$3p^53d^94d$,$3p^53d^95s$. The Slater integral factor is selected as 0.95. Because high order relativistic effect, the remnant correlation energy, the radiative corrections, the high order Breit effect and the quantum electrodynamics effect of high-Z ions are not considered in the Cowan's HFR program pack, we need to revise calculation results of the program using the fitting formula (3) proposed by us.

4 Results and discussion

Using the multi-configuration self-consistent field method together with the fitting formula (3) proposed by us, we have calculated energy levels, transitions and oscillator strength of highly ionized cobalt-like Cd^{21+} ions $3p^63d^9$,$3p^53d^{10}$,$3p^63d^84p$ configurations. The fitting parameters of energy level are shown in Table 1 and the fitting values of energy level are shown in

Table 1: Fitted parameter values of energy levels determined for cobalt-like Cd^{21+} ions.

JN_{th}	A	B	C	D	E	F	G	H
$3p^63d^9$								
$2D_{5/2}$	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
$2D_{3/2}$	-2024.91	604.141	-65.5063	2.92561	-0.4444955	0.00331144	-0.000526368	0.0000247112
$3p^53d^{10}$								
$2P_{1/2}$	-74732.66	26434.64	-2506.633	101.6266	-1.649258	0.113669	-0.01608	0.00525402
$2P_{3/2}$	-30246.8	15791.1	-1568.82	65.9696	-1.02663	0.0916599	-0.00671575	0.000224571
$3p^63d^84p$								
$4D_{3/2}$	28262400	-8087120	863323	-40771.4	718.979	-11.5441704	0.3443602	-0.01898167
$4P_{3/2}$	-2437540	694519	-74021.4	3497.43	-61.775	7.1548204	-0.15523201	0.0164119
$2D_{1/2}$	-69407	22603.4	-2769.81	149.716	-2.97499	0.2332896	-0.01101523	0.0257287
$2P_{1/2}$	6144790	-1711260	178648	-8271.72	143.367	-9.5390701	0.23643613	-0.0171815

Table 2. From Table 2, the difference values between fitting and experimental values are less than 50 cm^{-1}. It indicates that our theoretical calculation is successful. According to selection rules of configuration transition $\Delta J = J - J' = 0, \pm 1$ (except $J = J' = 0$), we have calculated the wavelengths of cobalt-like Cd^{21+} ions $3p^6 3d^9$–$3p^5 3d^{10}$, $3p^6 3d^9$–$3p^6 3d^8 4p$ transitions, which are shown in Table 3. From Table 3, the difference values between fitting and experimental values are less than 0.005 nm. It indicates that the datum in this paper are accurate.

In our results, the transitions of cobalt-like Cd^{21+} ions are not within Soft-X-Ray wavelength (2.33 nm–4.36 nm). It needs that we continue to calculate other cobalt-like ions or other isoelectronic sequence ions. At the present time, we don't find the datum of MCDF method about the wavelengths of cobalt-like Cd^{21+} ions $3p^6 3d^9$–$3p^5 3d^{10}$, $3p^6 3d^9$–$3p^6 3d^8 4p$ transitions. Although we don't find the transitions within Soft-X-Ray wavelength, our results will benefit the heavy ions reaction and scattering [18–21].

Table 2: Fitted $3p^6 3d^9$, $3p^5 3d^{10}$, $3p^6 3d^8 4p$ energy levels of cobalt-like Cd^{21+} ions (unit × 1000 cm^{-1}).

JN_{th}	E_{fit}	$E_{\text{fit-exp}}$
$3p^6 3d^9$		
$2D_{5/2}$	0.0	0.0
$2D_{3/2}$	58.2589	-0.0215
$3p^5 3d^{10}$		
$2P_{1/2}$	2203.1792	0.0257
$2P_{3/2}$	2076.0234	0.0241
$3p^6 3d^8 4p$		
$4D_{3/2}$	3784.8826	-0.0005
$4P_{3/2}$	3653.1676	0.0033
$2D_{1/2}$	3965.6131	0.0420
$2P_{1/2}$	3816.6917	-0.0012

Table 3: Fitted $3p^6 3d^9$–$3p^5 3d^{10}$, $3p^6 3d^9$–$3p^6 3d^8 4p$ transitions (unit: nm) and oscillator strengths of cobalt-like Cd^{21+} ions.

JN_{th}–JN_{th}	λ_{fit}	$\lambda_{\text{fit-exp}}$	gf
$3p^6 3d^9 - 3p^5 3d^{10}$			
$2D_{5/2} - 2P_{3/2}$	58.296	0.001	0.073
$2D_{3/2} - 2P_{1/2}$	51.251	-0.005	0.172
$2D_{3/2} - 2P_{3/2}$	60.345	-0.003	0.065
$3p^6 3d^9 - 3p^6 3d^8 4p$			
$2D_{5/2} - 4D_{3/2}$	16.531	0.003	0.501
$2D_{5/2} - 4P_{3/2}$	26.549	0.002	0.772
$2D_{3/2} - 4D_{3/2}$	21.654	0.001	0.452
$2D_{3/2} - 4P_{3/2}$	28.654	0.002	0.062
$2D_{3/2} - 2D_{1/2}$	27.754	-0.005	0.525
$2D_{3/2} - 2P_{1/2}$	27.124	-0.002	0.465

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