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ENERGY LEVELS, WAVELENGTHS, PROBABILITIES, AND OSCILLATOR STRENGTHS OF TRANSITION FOR Ge-LIKE Pd, Ag, and Cd IONS **

M. Wu^{1*}, Zh. He^{2,3}, F. Hu⁴

¹ Department of General Education, Anhui Xinhua University, Hefei Anhui 230088, China; e-mail: wumiao1121@163.com

² Shanghai EBIT Laboratory, Institute of Modern Physics, Shanghai 200433, China

³ Key Laboratory of Nuclear Physics and Ion-beam Application (MOE) at Fudan University, Shanghai 200433, China

⁴ School of Mathematic and Physical Science at Xuzhou University of Technology, Xuzhou 221111, Jiangsu, China

High-accuracy calculations of energy levels, wavelengths, probabilities, and oscillator strengths of transition of resonance lines for Ge-like Pd, Ag, and Cd ions have been performed. For the accurate treatment of relativity, the contributions of Breit interactions and quantum electrodynamics correction were considered. The calculated values of energy levels and wavelengths, including core-valence corrections, are found to be in excellent agreement with other theoretical and experimental values for Ge-like Pd, Ag, and Cd ions. The number of energy levels and wavelengths we considered is larger than that of any other theoretical calculations. The transition probabilities are also given where no other theoretical results and experimental values are available.

Keywords: multiconfiguration Dirac–Hartree–Fock, energy level, wavelength, transition probabilities, oscillator strength.

УРОВНИ ЭНЕРГИИ, ДЛИНЫ ВОЛН, ВЕРОЯТНОСТИ И СИЛЫ ОСЦИЛЛЯТОРОВ ПЕРЕХОДОВ ДЛЯ Ge-ПОДОБНЫХ ИОНОВ Pd, Ag и Cd

M. Wu^{1*}, Zh. He^{2,3}, F. Hu⁴

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¹Аньхойский университет Синьхуа, Хэфэй, Аньхой 230088, Китай; e-mail: wumiao1121@163.com

² Институт современной физики, Шанхай 2004336 Китай

³ Университет Фудань, Шанхай 200433, Китай

⁴ Школа математических и физических наук Технологического университета Сюйчжоу, Сюйчжоу 221111, Цзянсу, Китай

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Расчеты уровней энергии, длин волн, вероятностей и силы осцилляторов переходов резонансных линий для Ge-подобных ионов Pd, Ag, Cd выполнены в связи с необходимостью более точного учета релятивистских эффектов. Оценены вклады брейтовских взаимодействий и квантовой электродинамической коррекции. Уровни энергии и длины волн, вычисленные с учетом поправок на валентность ядра, находятся в хорошем согласии с другими теоретическими и экспериментальными данными для Ge-подобных ионов Pd, Ag, Cd. Количество рассмотренных энергетических уровней и длин волн больше, чем при любых других теоретических расчетах. Приведенные данные для вероятностей включают в себя переходы, для которых отсутствуют другие теоретические и экспериментальные результаты.

Ключевые слова: мультиконфигурация Дирака–Хартри–Фока, уровень энергии, длина волны, вероятность перехода, сила осциллятора.

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Introduction. Ions of the germanium isoelectronic sequence have four valence electrons outside a closed n = 3 core and provide a model for studying the effects of strong correlation on closely spaced levels in heavy atoms [1]. Theoretical predictions of atomic characteristics for highly ionized atomic systems is one of the important subjects in atomic physics during the past few years, which is important in many fields of science and technology such as laser physics, plasma physics, and astrophysics. However, experimental data and theoretical predictions on these systems are not sufficiently complete presently.

In the past few decades, many experimental and theoretical studies have been conducted for ions of the germanium isoelectronic sequence. In the experiments, the spectra of the germanium-like ions of Rb VI, Sr VII, Y VIII, Zr IX, Nb X, and Mo XI have been investigated in the region 280–790 Å by Litzén et al. [2]. The wavelengths of $4s^24p^2-4s4p^3$ transitions of Ge-like Ru and Rh ions have been measured in the range of 250–500 Å using laser-produced plasmas by Dunne et al. [3]. Lines of the resonance transition array $4s^24p^2-4s4p^3$ in the Ge-like ions of Ru XIII, RhXIV, PdXV, AgXVI, and CdXVII have been identified in spectra emitted from laser produced plasmas by Litzén et al. [4].

In terms of theoretical computation, transition probabilities are presented for the $4s^24p^2-4s^4p^3$ transitions of germanium-like ions ($37 \le Z \le 47$) using the method of relativistic Hartree-Fock by Biémont et al. [5]. Calculations for the ground and low-lying excited states of the $4s^24p^2$ configuration of germanium and Ge-like ions of As II, Se III, Br IV, and Kr V were performed using the relativistic multireference Møller-Plesset second-order perturbation theory by Ishikawa and Vilkas [6]. Wavelengths and transition probabilities of Ge-like ions with Z = 70-92 have been calculated using the fully relativistic multiconfiguration Dirac-Fock method (MCDF) by Palmeri et al. [7]. Energies of low-lying levels, transition energies, and rates of ground state transitions in Cu- through Ge-like ions of iodine have been calculated using the GRASP2K package by Li et al. [8]. Energy levels, wavelengths, transition probabilities, and oscillator strengths of Gelike Kr, Mo, Sn, and Xe ions among the fine-structure levels were calculated by Nagy and El-sayed [9]. The atomic structure and X-ray spectra of Ge-like through V-like W ions were calculated using the flexible atomic code (FAC) by Clementson et al. [10]. The energy levels, oscillator strengths, and transition probabilities for 4s-4p of Cu, Zn, Ga, and Ge-like gold ions were calculated using the fully relativistic MCDF method by Bian et al. [11]. The energy levels and lifetimes of the low-lying excited states of Ni- to Kr-like Pt ions were reported using the relativistic multi-reference Møller-Plesset many-body perturbation theory by Santana et al. [12]. Fine structure energy levels, transition probabilities, and oscillator strengths of germanium and Gelike ions (Z = 33-42) have been calculated using the Hartree-Fock method with relativistic correction by Wajid [13]. Energy levels, wavelengths, oscillator strengths, and transition probabilities of Ge-like ions with $49 \le Z \le 58$ among the lowest 88 fine structure levels belonging to the ([Ar]3d¹⁰)4s²4p², ([Ar]3d¹⁰)4s²4p4d, $([Ar]3d^{10})4s4p^3$, $([Ar]3d^{10})4s4p^24d$, $([Ar]3d^{10})4s^24d^2$, and $([Ar]3d^{10})4p^4$ configurations were calculated using the fully relativistic multiconfiguration Dirac-Fock (MCDF) approach by Chen and Wang [14]. The energy levels, wavelengths, transition rates, and line strengths have been calculated for the $4s^24p^2-4s^4p^3$ and $4s^24p^2-4s^24p4d$ allowed transitions of Ge-like Te, Xe, and Ba ions using MCDF by Hao et al. [15]. Energy levels, wavelengths, transition probabilities, and line strengths are calculated for the allowed electric dipole $4s^24p^2-4s^4p^3$ and $4s^24p^2-4s^24p^4d$ transitions of Ge-like ions with Z = 53, 55, and 57 using the fully relativistic multiconfiguration Dirac-Fock (MCDF) approach by Hao et al. [16]. However, atomic spectral data of highly charged Ge-like Pd, Ag, and Cd ions are still extremely scarce to date in the experimental and theoretical aspects.

The purpose of this work is to calculate the theoretical parameters (energy levels, wavelengths, transition probabilities, and oscillator strengths) of Ge-like Pd, Ag, and Cd ions using the multiconfiguration Dirac–Hartree–Fock (MCDHF) method systematically. In MCDHF the contributions from Breit interaction, vacuum polarization, self-energy, and finite nuclear mass corrections are taken into account. Comparisons are made with other experimental values and theoretical calculations, and good agreement is achieved for most of the results. In addition, the discrepancies with other theoretical and experimental values are also discussed in detail.

Method. Our calculations are based on the MCDHF method, which has particular advantage in dealing with highly charged ions with several valence electrons. Details about the theoretical method are in the monograph of Grant [17]. Here we only give a brief description of the method.

In the MCDHF method, an atomic state functions (ASF) ψ is fabricated by the linear combination of configuration state functions (CSFs) ϕ for a many electron atomic system:

$$\psi(\gamma P J M_J) = \sum_{i}^{n_c} c_i \phi(\gamma_i P J M_J), \qquad (1)$$

where c_i is the mixing coefficient for the state of *I*; γ represents other appropriate labeling of the CSF; *P* is the parity, *J* and *M_J* are total angular momentum and magnetic quantum number; n_c is the number of CSFs.

In the CSF, ϕ is constructed as an antisymmetrized linear combination of products of one-electron Dirac orbitals. The orbital is of the form

$$\phi(r) = \frac{1}{\mathbf{r}} \begin{pmatrix} P_{n\kappa}(r)\chi_{\kappa m}(\mathbf{r}) \\ iQ_{n\kappa}(r)\chi_{-\kappa m}(\mathbf{r}) \end{pmatrix}, \tag{2}$$

where *n*, κ , and *m* are the principal quantum number, the relativistic angular quantum number, and the magnetic quantum number respectively; $P_{n\kappa}(r)$ and $Q_{n\kappa}(r)$ are the large and small components of one-electron radial wavefunctions; $\chi_{\kappa m}(\mathbf{r})$ is the spinor spherical harmonic in a *LSJ*-coupling scheme.

In an N-electron atom or ion, all the dominant interactions are included in the Dirac-Coulomb Hamiltonian,

$$H_{DC} = \sum_{i}^{N} (c\alpha_{i} \bullet p_{i} + (\beta_{i} - 1)c^{2} + V_{i}) + \sum_{i < j}^{N} \frac{1}{r_{ij}}, \qquad (3)$$

where α_i and β_i are the Dirac matrices, p_i is the momentum of the electron, and V_i is the nuclear potential at radius *r*.

The contributions from Breit interaction, vacuum polarization, self-energy, and finite nuclear mass corrections are added as a first-order perturbation correction after self-consistency has been obtained. The transverse Breit interaction is

$$B_{ij} = -\frac{1}{2r_{ij}} \left[\alpha_i \bullet \alpha_j + \frac{(\alpha_i \bullet r_{ij})(\alpha_j \bullet r_{ij})}{r_{ij}^2} \right].$$
(4)

There are two major components in the QED correction. Known simply as self-energy, the dominant correction to energy arises from the lowest-order modification to an electron's interaction with quantized ambient electromagnetic field due to the nucleus and the other atomic electrons. In terms of a function E_{nk}^{SE} that varies slowly with respect to its argument, the self-energy in hydrogen like systems is given by

$$E_{nk}^{SE}(Z/c) = \frac{Z^4}{\pi c^3 n^3} F_{nk}(Z/c) .$$
(5)

Tabulations of $F_{nk}(Z/c)$ for the 1s, 2s, $2p_{1/2}$, and $2p_{3/2}$ states in these one-electron systems are given in the literature [18, 19]. In GRASP2K, a rough estimate of the self-energy is obtained by setting

$$H_{rr}^{SE}(Z/c) = \sum_{a=1}^{n_{0}} q_{r}(a) E_{n_{a}k_{a}}^{SE},$$

$$E_{n_{a}k_{a}}^{SE} = \frac{(Z_{a}^{eff})^{4}}{\pi c^{3} n^{3}} \begin{cases} F_{n_{a}k_{a}}(Z_{a}^{eff}/c) & \text{for } ns, np_{1/2} \text{ and } np_{3/2} \text{ orbital}, \\ F_{2k_{a}}(Z_{a}^{eff}/c) & \text{for } 1s, 2s, 2p_{1/2} \text{ and } 2p_{3/2} \text{ orbital}, \\ 0 & \text{other.} \end{cases}$$
(6)

The use of Z^{eff} for rough correction of electron screening is at best an expedient device intended for inner shells where the orbitals are most likely to be nearly hydrogenic. It is likely to be increasingly less realistic as *n* increases.

Next in order of importance is the vacuum polarization correction. To lowest order, this is the shortrange modification of the nuclear field due to screening by virtual electron positron pairs. Expressions for the second- and fourth-order perturbation potentials that take fine nuclear size into account have been given in the literature [20]. Only diagonal contributions

$$H_{rr}^{VP} = \sum_{a=1}^{n_{\omega}} q_r(a) \int_0^\infty dr V^{VP}(r) (P_{n_a k_a}^2(r) + Q_{n_a k_a}^2(r)) .$$
⁽⁷⁾

These potentials have been included in this version of GRASP2K.

All the calculations are done in the relativistic configuration interaction, where optimization is on a weighted sum of energies.

Once the ASFs are obtained, transition properties between two atomic states $\psi(\gamma P J M_J)$ and $\psi(\gamma' P' J' M'_J)$ can be expressed according to the reduced transition matrix element:

$$\left\langle \psi(\gamma P J M_J) \left\| Q_k^{(\lambda)} \right\| \psi(\gamma' P' J' M_J') \right\rangle.$$
(8)

Here $Q_k^{(\lambda)}$ is the transition operator in Coulomb or Babushkin gauge. The type of multipole transition is designated by superscript λ .

All the expanded configurations are generated by the active space approach, in which we consider electrons from the active space and core space, and these electrons are excited from occupied orbitals to unoccupied ones. The CSFs are increased systematically to guarantee the convergence of the atomic parameters calculated. Here, we refer to the $\{1s, 2s, 2p, ..., 4s, 4p, 4d, 4f\}$ set of orbitals as the n = 4 orbital layer and $\{1s, 2s, 2p, ..., 5s, 5p, 5d, 5f, 5g\}$ as n = 5, etc. To improve the calculations efficiently and ensure the accuracy of calculated values, we have chosen the active space set with the principal quantum number $n \le 1-8$ and $l \le 5$. For the studies of Ge-like ions, an argon-like core and four outer electrons are used. The active space is defined as follows:

$$AS1 = \{4s, 4p, 4d, 4f\}.$$
 (9)

Then the active set was increased as follows:

$$AS(i+1) = AS(i) + \{(i+4)s, (i+4)p, (i+4)d, (i+4)f(i+4)g\},$$
(10)

where i = 1, ..., 4, and n = i+4.

In this way, for Ge-like Pd, Ag, and Cd ions, we consider the valence-valence (VV) and core-valence (CV) correlations, The core electrons are the $1s^2 2s^2 2p^6 3s^2 3p^6 3d^{10}$, and the valence electrons are the $4s^2 4p^2$; the VV and CV correlation effects are taken into consideration systematically. The largest contribution is due to the CV correction from the 3*d*-orbitals, and the corrections from the 3*s*- and 3*p*-orbitals are very small. Thus, we only include the effect of polarization of the 3*d* core in the calculations [1, 21, 22]. We divide the reference configurations into even and odd parity in the calculation, which are $4s^2 4p^2$ and $4s 4p^3$, $4s^2 4p 4d$ configurations, and the energy levels were calculated as functions of increasing active sets with double (SD) excitations.

Results and discussion. The energy levels of Ge-like Pd ions have been tabulated in Table 1, where n represents the largest principal quantum number of the active set involved in each step of calculation. As can be seen from Table 1, the VV correlations have converged when n = 8, which is because the contribution from n = 8 is less than 0.02%. As for CV correlations, the principal number has been limited to n = 6 because the number of the CSFs increase very rapidly when we consider the 3d orbitals, so it is very difficult to get convergence. Also because of the computer calculation limit, we did not compare the VV and CV models on an equal footing. From Table 1, we can see that the core-valence correlation is important in determining the energy of the calculated levels, the CV results are found to be close to the Exp. [4] results, and the maximum difference is only 0.8%.

Key	T and a	Vale	nce-Valen	ce correct	ions	Core-V			
	Levels	<i>n</i> = 5	<i>n</i> = 6	<i>n</i> = 7	<i>n</i> = 8	<i>n</i> = 4	<i>n</i> = 5	n = 5 $n = 6$ Exp. 0 0 0 36480 36587 368 50069 50038 5000 98449 98386 982 135912 135509 1343 284489 284859 343968 343785	Exp.[4]
1	$4s^24p^2{}^3P_0$	0	0	0	0	0	0	0	0
2	$4s^24p^2{}^3P_1$	36238	36274	36296	36303	36231	36480	36587	36879
3	$4s^24p^2{}^3P_2$	49709	49713	49714	49716	50341	50069	50038	50024
4	$4s^24p^2 D_2$	97688	97687	97685	97687	98939	98449	98386	98299
5	$4s^24p^2 {}^1S_0$	134788	134682	134586	134565	137307	135912	135509	134394
6	$4s4p^{3}{}^{5}S_{2}$	281789	282118	282273	282308	282003	284489	284859	
7	$4s4p^{3}{}^{3}D_{1}$	342362	342572	342685	342702	343678	343968	343785	344280
8	$4s4p^{3}{}^{3}D_{2}$	346829	347062	347180	347200	348212	348849	348747	349448
9	$4s4p^{3}{}^{3}D_{3}$	361197	361445	361567	361588	362645	363338	363245	363993
10	$4s4p^{3}{}^{3}P_{0}$	393413	393540	393627	393639	395143	395171	394787	

 TABLE 1. Energy Levels (cm⁻¹) for Lower States of Ge-like Pd Ions as a Function of Increased Active Sets of Orbitals

		Pd XV				Ag XVI	Cd XVII		
Key	levels	CV	Exp.[4]	Ref.[5]	CV	Exp.[4]	Ref.[5]	CV	Exp.[4]
1	$4s^24p^2{}^3P_0$	0	0	0	0	0	0		0
2	$4s^2 4p^2 {}^3P_1$	36587	36879	37047	43066	43364	43648	50279	50622
3	$4s^24p^2{}^3P_2$	50038	50024	50272	57413	57366	57741	65493	65490
4	$4s^24p^2 {}^1D_2$	98386	98299	98492	112656	112548	112914	128382	128378
5	$4s^24p^2 {}^1S_0$	135509	134394	134456	151180	150039	150226	168304	
6	$4s4p^{3}{}^{5}S_{2}$	284859		289253	308770		312570	333415	
7	$4s4p^{3}{}^{3}D_{1}$	343784	344280	343797	369587	369836	369187	396072	396359
8	$4s4p^{3}{}^{3}D_{2}$	348747	349448	349229	376549	377080	376782	405595	406214
9	$4s4p^{3}{}^{3}D_{3}$	363245	363993	363517	393338	393860	393266	424760	425385
10	$4s4p^{3}{}^{3}P_{0}$	394787		394668	426189		425858	458921	
11	$4s4p^{3}{}^{3}P_{1}$	400273	400398	400238	432670		432385	466466	
12	$4s4p^{3}{}^{3}P_{2}$	405519	405862	405407	438394	438459	437875	472562	472709
13	$4s4p^{3}D_{2}$	448173	448370	447731	485099	485082	484207	523932	524051
14	$4s4p^{3}{}^{3}S_{1}$	451811	451084	450706	484305	483331	482802	518029	517151
15	$4s4p^{3} P_1$	506754	506044	505673	546991	545974	545601	589147	588233
16	$4s^24p4D {}^3F_2$	515044			550014			585538	
17	$4s^24p4D {}^3F_3$	535019			572790			611274	
18	$4s^24p4D \ ^3P_2$	559538			597313			635724	
19	$4s^24p4D \ ^3D_1$	570428			608161			646362	
20	$4s^24p4D \ ^1D_2$	594724			637993			682472	
21	$4s^24p4D {}^3P_0$	602826			646599			691539	
22	$4s^24p4D {}^3P_1$	607663			651868			697289	
23	$4s^24p4D \ ^3D_3$	609270			653168			698208	
24	$4s^24p4D \ ^3D_2$	613566			658625			705021	
25	$4s^24p4D {}^1F_3$	652828			699284			746953	
26	$4s^24p4D \ ^1P_1$	662420			709626			758112	
27	$4p^{4}{}^{3}P_{2}$	709853			758520			808680	
28	$4p^{4}{}^{3}P_{0}$	741447			792881			845793	
29	$4p^{4} {}^{3}P_{1}$	752695			808158			865492	
30	$4p^{4} D_2$	761973			817841			875752	

TABLE 2. Comparison of the Energy Levels (cm⁻¹) Calculated with Available Experimental and Theoretical Values of Ge-like Pd, Ag, and Cd Ions

In Table 2, the calculated energy levels of Pd XV, Ag XVI, Cd XVII were compared with the experimental value [4] and the values of previous calculations [5] using the relativistic Hartree–Fock method. "CV" indicates that core-orbital correlations are included. From Table 2, for the ions of Pd XV, we can see that our MCDHF results are in good agreement with the value of experiment. The maximum discrepancy between our calculated energies and experimental value is less than 0.8%. The results of our calculations agree well with the theoretical values calculated by others [5], and the discrepancies are within 1% except for the state of $4s4p^{3}5S_{2}$ (1.5%). For the ions of Ag XVI, the major part of $4s^{2}4p^{2}$, $4s4p^{3}$, our results are closer to the experimental values than those of other theoretical calculations. The maximum discrepancy between our calculated energies and experiment is also less than 0.8%. For the ions of Cd XVII, our MCDHF results are in good agreement with the experimental values; there are no other theoretical values. Therefore, we can conclude that the configuration interactions we considered are enough to describe the system of Pd XV, Ag XVI, Cd XVII. The excited states of $4s^{2}4p4d$, $4p^{4}$ of Pd XV, Ag XVI, and Cd XVII are also calculated and listed in Table 2. For these excited states, there are no other theoretical or experimental values so far. The excited states of Pd XV, Ag XVI, and Cd XVII are important in nuclear fusion research as the spectra of these ions may provide diagnostic information on magnetically confined plasmas.

Wavelengths of the Ge-like Pd, Ag, and Cd ions were calculated and are listed in Tables 3 and 4. Other theoretical results and experimental value are also displayed to illustrate the accuracy of the calculated results. In Table 3, the calculated wavelengths for Ge-like Pd, Ag, and Cd ions are compared with experimental wavelengths by Litzén and Zeng [4] and with theoretical results by Biémont et al. [5]. As can be seen

Lower state	Upper state		Pd XV		Ag XVI			Cd XVII		
		λ, Å	Ref.[5]	Exp.[4]	λ, Å	Ref.[5]	Exp.[4]	λ, Å	Exp.[4]	
$4s^24p^2{}^3P_0$	$4s4p^{3}{}^{3}D_{1}$	290.88	290.87	290.46	271.42	270.87	270.39	252.48	252.30	
$4s^2 4p^2 {}^3P_0$	$4s4p^{3}S_{1}$	221.33	221.87	221.67	203.94	207.12	206.88	193.04	193.34	
$4s^24p^2{}^3P_1$	$4s4p^{3}{}^{3}S_{1}$	240.83	241.75	241.43	223.45	227.71	227.29	213.79	214.35	
$4s^24p^2{}^3P_1$	$4s4p^{3}{}^{3}D_{2}$	320.35	320.32	319.93	301.20	300.18	299.66	281.44	281.22	
$4s^24p^2{}^3P_2$	$4s4p^{3}{}^{3}S_{1}$	248.90	249.73	249.33	230.79	235.26	234.76	220.98	221.40	
$4s^24p^2 D_2$	$4s4p^{3} P_1$	244.88	245.59	245.25	227.45	231.11	230.72	217.03	217.46	
$4s^24p^2{}^3P_2$	$4s4p^{3}{}^{3}P_{2}$	281.31	281.58	281.03	262.75	263.05	262.41	245.66	245.57	
$4s^24p^2 {}^1D_2$	$4s4p^{3} D_2$	285.89	286.33	285.66	267.99	269.32	268.42	252.81	252.73	
$4s^24p^2{}^3P_2$	$4s4p^{3}{}^{3}D_{3}$	319.28	319.24	318.50	298.97	298.04	297.18	278.34	277.86	
$4s^24p^2 D_2$	$4s4p^{3}{}^{3}D_{3}$	377.56	377.32	367.37	357.60	356.69	355.48	337.41	336.69	
$4s^24p^2 {}^1S_0$	$4s4p^{3} P_{1}$	269.36	269.38	269.07	249.10	252.92	255.56	237.62		
$4s^24p^2{}^3P_2$	$4s4p^{3} D_2$	251.17	251.60	251.03	233.66	234.49		218.13		
$4s^24p^2{}^3P_1$	$4s4p^{3}{}^{3}P_{1}$	274.96	275.33	275.08	257.21	257.24		240.28		
$4s^24p^2{}^3P_2$	$4s4p^{3}{}^{3}D_{2}$	334.77	334.50		314.68	313.44		294.03		
$4s^24p^2{}^3P_1$	$4s4p^{3}{}^{3}P_{2}$	271.05	271.47		253.28	253.66		236.81		
$4s^24p^2{}^3P_2$	$4s4p^{3}{}^{3}D_{1}$	340.43	340.68		321.14	321.08		302.50		
$4s^24p^2{}^3P_2$	$4s4p^{3}{}^{3}P_{1}$	285.52	285.74		266.99	266.92		249.39		
$4s^24p^2{}^3P_1$	$4s4p^{3} P_{1}$	212.69	213.39		196.57	199.22		185.57		
$4s^24p^2{}^3P_1$	$4s4p^{3}{}^{3}P_{0}$	279.17	279.62		261.76	261.63		244.71		
$4s^2 4p^2 {}^3P_1$	$4s4p^{3}{}^{3}D_{1}$	325.52	325.99		307.11	307.18		289.19		
$4s^24p^2{}^3P_0$	$4s4p^{3} P_1$	197.33	197.76		181.31	183.28		169.74		
$4s^2 4p^2 {}^3P_0$	$4s4p^{3} {}^{3}P_{1}$	249.83	249.85		231.70	231.28		214.38		
$4s^2 4p^2 {}^1S_0$	$4s4p^{3}S_{1}$	316.15	316.20		293.91	300.68		285.94		

TABLE 3. Comparison of Calculated with Experimental and Theoretical Wavelengths (Å) of $4s^24p^2-4s4p^3$ Transition for Ge-like Pd, Ag, and Cd ions

TABLE 4. Wavelengths (Å) of $4s^24p^2-4s^4p^3$ and $4s^24p^2-4s^24p^4d$ Transition
for Ge-like Pd, Ag, and Cd Ions

Lower state	Upper state	Pd XV	AgXVI	CdXVII	Lower state	Upper state	PdXV	AgXVI	PdXVII
$4s^24p^2{}^3P_1$	$4s4p^{3}{}^{5}S_{2}$	402.78	379.70	353.19	$4s^24p^2 D_2$	$4s^24p4D {}^3F_2$	240.01	228.46	218.74
$4s^24p^2 {}^1S_0$	$4s4p^{3}{}^{3}D_{1}$	480.13	458.01	439.04	$4s^24p^2 D_2$	$4s^24p4D {}^3P_2$	216.85	204.67	197.11
$4s^24p^2 {}^1S_0$	$4s4p^{3} {}^{3}P_{1}$	377.69	355.24	335.39	$4s^24p^2 D_2$	$4s^24p4D \ ^1D_2$	201.48	188.95	180.48
$4s^24p^2 D_2$	$4s4p^{3}{}^{5}S_{2}$	536.27	514.68	487.73	$4s^24p^2 D_2$	$4s^24p4D \ ^3D_2$	194.11	181.81	173.42
$4s^24p^2 D_2$	$4s4p^{3}{}^{3}D_{2}$	399.42	380.31	360.73	$4s^24p^2{}^3P_2$	$4s^24p4D {}^3F_2$	215.05	203.03	192.29
$4s^24p^2 D_2$	$4s4p^{3}{}^{3}P_{2}$	325.59	306.98	290.55	$4s^24p^2 {}^3P_2$	$4s^24p4D \ ^3P_2$	196.27	184.02	175.37
$4s^24p^2{}^3P_2$	$4s4p^{3}P_{1}$	218.95	202.23	190.97	$4s^24p^2 {}^3P_2$	$4s^24p4D \ ^1D_2$	183.59	171.21	162.08
$4s^24p^2 D_2$	$4s4p^{3}{}^{3}D_{1}$	407.50	389.79	373.57	$4s^24p^2{}^3P_2$	$4s^24p4D \ ^3D_2$	177.45	165.33	156.37
$4s^24p^2 D_2$	$4s4p^{3}{}^{3}P_{1}$	331.25	312.78	295.78	$4s^24p^2 {}^3P_2$	$4s^24p4D {}^3F_3$	206.19	194.16	183.22
$4s^24p^2 D_2$	$4s4p^{3}{}^{3}S_{1}$	282.95	264.23	256.64	$4s^24p^2 {}^3P_2$	$4s^24p4D \ ^3D_3$	178.82	166.69	158.05
$4s^24p^2{}^3P_1$	$4s4p^{3} D_2$	242.96	226.14	211.12	$4s^24p^2{}^3P_2$	$4s^24p4D {}^1F_3$	165.90	154.88	146.74
$4s^24p^2{}^3P_2$	$4s4p^{3}{}^{5}S_{2}$	425.86	401.39	373.24	$4s^24p^2 D_2$	$4s^24p4D {}^3F_3$	229.03	217.30	207.09
$4s^24p^2{}^3P_1$	$4s^24p4D \ ^1P_1$	159.79	149.47	141.28	$4s^24p^2 D_2$	$4s^24p4D \ ^3D_3$	195.74	183.46	175.49
$4s^24p^2{}^3P_1$	$4s^24p4D {}^3F_2$	209.01	197.33	186.83	$4s^24p^2 D_2$	$4s^24p4D {}^1F_3$	180.36	169.25	161.66
$4s^24p^2{}^3P_1$	$4s^24p4D \ ^3P_2$	191.22	179.32	170.81	$4s^24p^2 {}^3P_0$	$4s^24p4D \ ^3D_1$	175.31	163.42	154.71
$4s^24p^2{}^3P_1$	$4s^24p4D \ ^1D_2$	179.17	167.13	158.18	$4s^24p^2{}^3P_0$	$4s^24p4D {}^3P_1$	164.56	152.73	143.41
$4s^24p^2{}^3P_1$	$4s^24p4D \ ^3D_2$	173.32	161.53	152.73	$4s^24p^2{}^3P_0$	$4s^24p4D \ ^1P_1$	150.96	140.48	131.91
$4s^24p^2{}^3P_2$	$4s^24p4D \ ^3D_1$	192.16	180.22	172.16	$4s^24p^2 {}^1S_0$	$4s^24p4D \ ^3D_1$	229.93	216.53	209.18
$4s^24p^2{}^3P_2$	$4s^24p4D \ ^3P_1$	179.33	167.31	158.28	$4s^24p^2 {}^1S_0$	$4s^24p4D {}^3P_1$	211.80	198.16	189.04
$4s^24p^2{}^3P_2$	$4s^24p4D \ ^1P_1$	163.30	152.72	144.38	$4s^24p^2 {}^1S_0$	$4s^24p4D \ ^1P_1$	189.79	178.01	169.55
$4s^24p^2 D_2$	$4s^24p4D \ ^3D_1$	211.85	199.98	193.06	$4s^24p^2 {}^3P_1$	$4s^24p4D {}^3P_0$	176.60	164.99	155.94
$4s^24p^2 D_2$	$4s^24p4D \ ^3P_1$	196.36	184.21	175.78	$4s^24p^2 {}^3P_1$	$4s^24p4D \ ^3D_1$	187.32	175.71	167.76
$4s^24p^2 D_2$	$4s^24p4D \ ^1P_1$	177.29	166.67	158.80	$4s^24p^2{}^3P_1$	$4s^24p4D {}^3P_1$	175.11	163.42	154.56

from Table 3, for the transition of $4s^24p^2-4s4p^3$, our results are in good agreement with theoretical values by Biémont et al. [5] and the experimental value [4] for the Ge-like Pd ions, which is the same as Ge-like Ag ions except for the transition of ${}^{3}P_{J}-{}^{3}S_{1}$, ${}^{1}D_{2}-{}^{1}P_{1}$, ${}^{1}S_{0}-{}^{1}P_{1}$, where the maximum error is less than 2%. For the Ge-like Cd ions, there are no other theoretical values, and our calculated results are in good agreement with the experimental values. The good agreements above show that our calculated results are accurate and reliable. Some other transition wavelengths of $4s^24p^2-4s4p^3$ and $4s^24p^2-4s^24p4d$ without experimental and theoretical values for Ge-like Pd, Ag, and Cd ions are also listed in Table 4.

In addition, the transition probabilities and oscillator strengths for the transition of $4s^24p^2-4s4p^3$ for Gelike Pd, Ag, and Cd ions with CV correction are listed in Table 5. They were calculated in both length and velocity form. We only show the calculated results in length form because the length form is more stable than the velocity form. We also provide other theoretical values obtained by Biémont et al. [5]. From Table 5, we can clear see that the calculated oscillator strengths of Ge-like Pd and Ag ions are in good agreement with the value of Biémont [5], except for the transition of ${}^{1}D_{2}-{}^{1}D_{2}$, ${}^{3}P_{2}-{}^{3}P_{2}$, ${}^{3}P_{1}-{}^{3}P_{2}$, where the maximum error reaches 27%. For the Ge-like Cd ions, there are no experimental and theoretical values to compare. The difference in the two calculation methods is the reason for the large disagreement in results. Unfortunately, there are no experimental results to compare.

 TABLE 5. Transition Probabilities and Oscillator Strengths for E1 Transitions of the Ge-like Pd, Ag, and Cd Ions

Lower	Upper	Pd XV			A	g XVI	Cd XVII		
state	state	A, s ⁻¹	log(gf)	Ref.[5]	A, s^{-1}	log(gf)	Ref.[5]	A, s^{-1}	log(gf)
$4s^24p^{23}P_0$	$4s4p^{3}{}^{3}D_{1}$	7.23D+09	-0.56	-0.52	8.78D+09	-0.54	-0.50	1.06D+10	-0.52
$4s^2 4p^2 {}^3P_0$	$4s4p^{3}P_{1}$	2.33D+09	-1.18	-1.18	2.62D+09	-1.20	-1.20	2.94D+09	-1.22
$4s^2 4p^2 {}^3P_0$	$4s4p^{3}{}^{3}S_{1}$	1.02D+10	-0.65	-0.63	1.13D+10	-0.66	-0.64	1.24D+10	-0.68
$4s^2 4p^2 {}^3P_0$	$4s4p^{3}P_{1}$	1.60D+09	-1.55	-1.54	1.93D+09	-1.54	-1.52	2.39D+09	-1.51
$4s^2 4p^2 {}^1S_0$	$4s4p^{3}{}^{3}S_{1}$	1.16D+09	-1.28	-1.18	1.31D+09	-1.27	-1.18	1.49D+09	-1.26
$4s^2 4p^2 {}^1S_0$	$4s4p^{3}P_{1}$	9.36D+09	-0.51	-0.46	1.04D+10	-0.52	-0.47	1.16D+10	-0.53
$4s^2 4p^2 {}^3P_1$	$4s4p^{3}{}^{3}P_{0}$	1.09D+10	-0.89	-0.87	1.25D+10	-0.89	-0.87	1.42D+10	-0.89
$4s^2 4p^2 {}^3P_1$	$4s4p^{3}{}^{3}D_{1}$	3.54D+07	-2.77	-2.77	1.12D+07	-3.32	-3.37	2.92D+05	-4.96
$4s^2 4p^2 {}^3P_1$	$4s4p^{3}{}^{3}P_{1}$	1.01D+10	-0.46	-0.43	1.22D+10	-0.44	-0.41	1.47D+10	-0.42
$4s^24p^2{}^3P_1$	$4s4p^{3}{}^{3}S_{1}$	1.96D+10	-0.29	-0.27	2.12D+10	-0.31	-0.29	2.28D+10	-0.33
$4s^2 4p^2 {}^3P_1$	$4s4p^{3}P_{1}$	1.33D+10	-0.57	-0.52	1.51D+10	-0.57	-0.53	1.70D+10	-0.58
$4s^2 4p^2 {}^3P_1$	$4s4p^{3}{}^{3}D_{2}$	4.43D+09	-0.47	-0.43	4.96D+09	-0.48	-0.44	5.52D+09	-0.48
$4s^2 4p^2 {}^3P_1$	$4s4p^{3}P_{2}$	6.59D+06	-3.44	-3.87	5.62D+04	-5.57	-4.04	1.10D+07	-3.33
$4s^2 4p^2 {}^3P_2$	$4s4p^{3}{}^{3}D_{1}$	4.83D+08	-1.60	-1.53	6.85D+08	-1.50	-1.44	9.47D+08	-1.41
$4s^2 4p^2 {}^3P_2$	$4s4p^{3}{}^{3}P_{1}$	6.35D+08	-1.63	-1.58	6.49D+08	-1.68	-1.64	6.61D+08	-1.73
$4s^2 4p^2 {}^3P_2$	$4s4p^{3}{}^{3}S_{1}$	5.10D+10	0.15	0.18	5.63D+10	0.14	0.16	6.20D+10	0.13
$4s^2 4p^2 D_2$	$4s4p^{3}P_{1}$	4.94D+10	0.12	0.15	5.47D+10	0.12	0.14	6.04D+10	0.11
$4s^2 4p^2 {}^3P_2$	$4s4p^{3}{}^{3}D_{2}$	8.52D+07	-2.15	-2.10	1.20D+08	-2.05	-2.03	1.57D+08	-1.99
$4s^24p^2{}^3P_2$	$4s4p^{3}{}^{3}P_{2}$	1.27D+10	-0.12	-0.08	1.51D+10	-0.11	-0.07	1.78D+10	-0.09
$4s^2 4p^2 {}^3P_2$	$4s4p^{3} D_2$	2.18D+09	-0.99	-0.93	2.10D+09	-1.06	-1.03	1.91D+09	-1.16
$4s^2 4p^2 D_2$	$4s4p^{3}D_{2}$	1.47D+10	-0.04	0.01	1.59D+10	-0.06	-0.02	1.71D+10	-0.09
$4s^24p^2{}^3P_2$	$4s4p^{3}{}^{3}D_{3}$	2.45D+09	-0.58	-0.53	2.73D+09	-0.60	-0.55	3.03D+09	-0.61
$4s^24p^2 D_2$	$4s4p^{3}{}^{3}D_{3}$	1.18D+09	-0.75	-0.69	1.40D+09	-0.73	-0.68	1.65D+09	-0.70
$4s^24p^2{}^3P_1$	$4s4p^{3}{}^{5}S_{2}$	2.47D+08	-1.52		3.52D+08	-1.43		4.86D+08	-1.34
$4s^2 4p^2 {}^3P_2$	$4s4p^{3}P_{1}$	3.63D+07	-3.11		1.00D+08	-2.72		2.03D+08	-2.48
$4s^2 4p^2 D_2$	$4s4p^{3}{}^{3}D_{1}$	2.33D+08	-1.76		2.59D+08	-1.75		2.79D+08	-1.76
$4s^2 4p^2 D_2$	$4s4p^{3}{}^{3}P_{1}$	8.96D+06	-3.35		4.79D+05	-4.68		3.96D+06	-3.81
$4s^24p^2 D_2$	$4s4p^{3}{}^{3}S_{1}$	5.56D+08	-1.70		7.78D+08	-1.60		1.04D+09	-1.51
$4s^24p^2{}^3P_2$	$4s4p^{3}{}^{5}S_{2}$	1.86D+08	-1.60		2.53D+08	-1.52		3.36D+08	-1.45
$4s^24p^2 D_2$	$4s4p^{3}{}^{5}S_{2}$	1.50D+07	-2.49		1.87D+07	-2.44		2.21D+07	-2.40
$4s^24p^2 D_2$	$4s4p^{3}{}^{3}D_{2}$	5.56D+07	-2.18		6.81D+07	-2.13		8.46D+07	-2.08
$4s^24p^2 D_2$	$4s4p^{3}{}^{3}P_{2}$	2.08D+08	-1.78		3.47D+08	-1.61		5.43D+08	-1.46

Conclusions. In this paper we report on the relativistic multiconfiguration Dirac–Hartree–Fock method of energy levels, wavelengths, and the transition probabilities of the Ge-like Pd, Ag, and Cd ions. We conclude that the energy levels obtained by considering the CV correlation agree well with the experimental and other theoretical values. Some new and previously unpublished energy levels, wavelengths, transition probabilities, and oscillator strengths for the Ge-like Pd, Ag, and Cd ions have been obtained. We hope that these results will be beneficial in analyzing previous experiments and planning new ones.

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