ENERGIES AND SPECTRAL LINES FOR THE STATES OF $4s^24p^2$, $4s4p^3$, and $4s^24p4d$ CONFIGURATIONS IN Ge-LIKE Te, Xe, and Ba IONS**

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The energy levels, wavelengths, transition rates, and line strengths have been calculated for the $4s^24p^2$–$4s4p^3$ and $4s^24p^2$–$4s^24p4d$ allowed transitions occurring within the ground configuration ($4s^24p^2$) in the heavy Ge-like Te, Xe, and Ba ions. The fully relativistic multiconfiguration Dirac–Hartree–Fock method taking into account both correlations within the n = 5 complex and the QED effects has been used in the calculations. The calculation results are found to agree well with the data obtained on the TFR tokamak and by recent EBIT measurements in Xe. The isoelectronic sequence of the Ge-like ions is important in nuclear fusion research as their spectra may provide diagnostic information on magnetically confined plasmas.

Keywords: *energy level, wavelength, transition rate, line strength.*

ЭНЕРГЕТИЧЕСКИЕ УРОВНИ И СПЕКТРАЛЬНЫЕ ЛИНИИ ПЕРЕХОДОВ В КОНФИГУРАЦИЯХ $4s^24p^2$, $4s4p^3$, $4s^24p4d$ Ge-ПОДОБНЫХ ИОНОВ Te, Xe, Ba

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Рассчитаны уровни энергии, длины волн, вероятности переходов и интенсивности линий для разрешенных переходов $4s^24p^2$–$4s4p^3$ и $4s^24p^2$–$4s^24p4d$ в основное состояние ($4s^24p^2$) тяжелых Ge-подобных ионов Te, Xe и Ba. Для расчета использован полностью релятивистский многоконфигурационный метод Дирака–Хартри–Фока, учитывающий как корреляции в комплексе n = 5, так и эффекты квантовой электродинамики. Результаты расчета удовлетворительно согласуются с данными, полученными на токамаке TFR, и результатами недавних измерений с ионной ловушкой электронных пучков в Xe. Рассмотренная изоэлектронная последовательность Ge-подобных ионов играет важную роль в исследованиях термоядерного синтеза, где их спектры могут обеспечить диагностическую информацию о плазме с магнитным удержанием.

Ключевые слова: *уровень энергии, длина волны, вероятность перехода, интенсивность линии.*

Introduction. Theoretical predictions of atomic characteristics for highly ionized atomic systems have been one of the important subjects in atomic physics during the past few years because knowledge of the structure and other properties of these systems is important in many fields of science and technology, such as plasma physics, laser physics, and astrophysics. However, experimental data on these systems are not sufficiently complete presently. In general, one has to use reliable theoretical predictions as input in other fields [1, 2]. Different relativistic many-body approaches have been successfully developed, and these include, for example, the self-consistent field method, the relativistic many-body perturbation theory (MBPT) [3], and the multiconfiguration Dirac–Fock (MCDF) [4], or the coupled-cluster (CC) approaches [5]. Semi-empirical

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techniques, like the relativistic multi-configuration Hartree–Fock approach (MCHF), have also extended considerably their range of applicability. As a consequence, it is now possible to predict term energies and radiation parameters such as wavelengths with unprecedented accuracy. However, radiative parameters of highly charged ions along the germanium isoelectronic sequence are still urgently needed from both theory and experiment. Highly charged Ge-like ions are interesting in this context because having several electrons outside closed shells, they allow us to test the predictive power of the theoretical models, which must include, in a reliable way, both relativity and correlation effects.

Transition probabilities and oscillator strengths for the $4s^24p^2$–$4s4p^3$ transitions of the Ge-like ions with ($37 \leq Z \leq 47$) have been studied by Biémont et al. [6]. Lines of the resonance transition array $4s^24p^2$–$4s4p^3$ in the Ge-like ions Ru XIII, Rh XIV, Pd XV, Ag XVI, and Cd XVII have been identified in the spectra emitted from laser-produced plasmas by Litzén and Zeng [7]. The energies of the low-lying levels, and the transition energies and rates of the ground state transitions in the Ge-like ions of iodine have been calculated in [8]. Energy levels, wavelengths, transition probabilities, and oscillator strengths for the Ge-like Kr, Mo, Sn, and Xe ions have been calculated by Nagy and El-Sayed [9]. Wavelengths and transition probabilities for the $4s^24p^2$–$4s4p^3$ and $4s^24p^2$–$4s^24p4d$ allowed ($E1$) transitions and for the $4s^24p^2$–$4s^24\mathrm{p}^2$ forbidden ($M1$ and $E2$) transitions have been calculated in the heavy Ge-like ions with Z = 70–92 by Palmeri et al. [10]. Spectra of the Ge-like ions Rb VI, Sr VII, Y VIII, Zr IX, Nb X, and Mo XI have been investigated in the region of 280–790 Å by Litzén and Reader [11]. The Xe spectrum in the 95–260 Å spectral region, excited in TFR tokamak plasmas, has been recorded by Breton et al. [12]. Extreme ultraviolet (EUV) spectroscopy of the highly charged Rb-like Xe^{17+} to Cu-like Xe^{25+} ions have been registered and identified by Biedermann et al. [13], calculating the atomic structure with the HULLAC code. EUV beam-foil observations of the Cu-through Ge-like ions of iodine have been performed by Träbert [14]. Also, EUV spectra of Sn XIX to Sn XXII observed in low-density plasmas have been compared with the theoretical calculations by Suzuki et al. [15]. So far, no theoretical and experimental data are available for the ions of Te and Ba along the Ge sequence. It is now well established that the energies and transition rates of these lines are of importance in various spectroscopic applications in plasma physics, fusion plasmas, and also in the study of atomic collisions, which in turn motivate us to calculate energies, wavelengths, radiative transition rates, and line strengths in the Ge-like Te, Xe, and Ba ions using the multiconfiguration Dirac–Hartree–Fock (MCDHF) code.

In the present work, we report energy level, wavelengths, transition rates, and line strengths for the $4s^24p^2$–$4s4p^3$ and $4s^24p^2$–$4s^24p4d$ allowed transitions occurring within the ground configuration ($4s^24p^2$) in the heavy Ge-like ions with Z = 52 to 56, Te XXI, Xe XXIII, and Ba XXV. We provide these new data to help line identifications in future experiments. The present results are compared to and agree well with the TFR tokamak and recent EBIT measurements in Xe.

Calculation. These calculations are performed using the fully relativistic MCDHF approach with the multiconfiguration Dirac–Hartree–Fock and General Matrix Elements (MCDFGME) [16] program in the form of the GRASP2K package [17]. We use a Dirac–Coulomb version for the optimization of the orbitals and include Breit corrections, quantum electrodynamics (QED), and nuclear mass corrections in the calculation of the final relativistic configuration interaction (RCI). We divide the calculations into two parts, where we optimize the sets of orbitals for even and odd states separately. Thus the upper and lower states are described by two independently optimized sets of orbitals. Because of this we have to use the biorthogonal transformation [18] of the atomic state functions to calculate the transition parameters.

The valence-valence (VV) and core-valence (CV) correlation effects are taken into account in a systematic way. We define a CV approach. Basically, we would like to include the effect of polarization of the 3d core, which to the first order can be represented by substitutions to the orbitals with l = 0–3. In a system as complex as the Ge-like ions, we need to start with a relatively good overall representation of the energy level structure before adding the core effects. We choose building the n = 5 step in the VV calculations. Let us briefly outline the main steps in these calculations. We start by optimizing all orbitals on the full active space of the CV correlation CSFs (including all l values): $3d^{10}\{4\}^4$.

When deriving the specific form of solving the MCDHF equations, we start by applying the variational principal to a functional of energy. It is common to use an extended optimal level (EOL) technique, where a linear combination of the most important energy levels is used. In the next step we generate all CSFs of the form $3d^9\{3,4\}\{4,5\}^1\{3,4,5\}^1$ with the constraint of only orbitals with $l \leq 3$.

In the final step, we include more VV by adding to the restricted active spaces all CSFs of the form $3d^{10}\{4,5\}\{4,5,6\}^2$ with $l \neq 3$, and optimize the orbitals $5f$, $6s$, $6p$, and $6d$.

Finally, the contributions from Breit interaction, quantum electrodynamics (QED), and nuclear mass corrections are taken into account. After obtaining the set of radial functions, we carry out the RCI calculations to determine CSF expansion coefficients by diagonalizing the Hamiltonian matrix that includes the frequency-dependent Breit interaction, vacuum polarization, and self-energy correction. In this implementation of the RCI program, an iterative Davidson method is used together with a spare matrix representation allowing for large expansions.

Results and discussion. The energy level values obtained using the MCDHF method for the $4s^24p^2$, $4s4p^3$, and $4s^24p4d$ configurations in the Ge-like Te, Xe, and Ba heavy ions are presented in Tables 1 and 2. For the reader's convenience, we also list the dominant configuration in the *LS*- and *jj*-coupling schemes, respectively. In our notation, the asterisk superscript * corresponds to the case of $j = l - 1/2$ while no superscript is given for $j = l + 1/2$. For such highly ionized atoms, the *jj*-coupling results appear to be much more adequate than those from the *LS*-coupling scheme.

TABLE 1. MCDHF Energy Levels of $4s^24p^2$, $4s4p^3$, and $4s^24p4d$ Configurations for Xe XXIII

Index	*jj*-coupling	*J*	$(LS)^p$	MCDHF, cm^{-1}	MCDF [9]
1	$4s^24p^{*2}$	0	$^3P_0^e$	0	0
2	$4s^24p^*4p$	1	$^3P_1^e$	112495	115319
3	$4s^24p^*4p$	2	$^3P_2^e$	133100	134513
4	$4s^24p^2$	2	$^1D_2^e$	261560	265682
5	$4s^24p^2$	0	$^1S_0^e$	311162	307412
6	$4s4p^{*2}4p$	2	$^5S_2^o$	503024	498050
7	$4s4p^{*2}4p$	1	$^3D_1^o$	578502	586888
8	$4s4p^{*2}4p$	2	$^3D_2^o$	619946	632798
9	$4s4p^24p^*$	3	$^3D_3^o$	654323	672642
10	$4s4p^24p^*$	0	$^3P_0^o$	697147	703903
11	$4s4p^24p^*$	1	$^3P_1^o$	711995	718420
12	$4s4p^3$	2	$^3P_2^o$	717583	739885
13	$4s4p^24p^*$	1	$^3S_1^o$	760151	759075
14	$4s4p^24p^*$	2	$^1D_2^o$	812118	843980
15	$4s4p^3$	1	$^1P_1^o$	900147	907508
16	$4s^24p^*4d^*$	2	$^3F_2^o$	833697	810264
17	$4s^24p^*4d$	3	$^3F_3^o$	872823	868044
18	$4s^24p^*4d^*$	1	$^3P_1^o$	906407	
19	$4s^24p^*4d^*$	2	$^3P_2^o$	912451	
20	$4s^24p4d$	4	$^3F_4^o$	969981	970144
21	$4s^24p4d$	2	$^1D_2^e$	1004543	974316
22	$4s^24p4d$□	0	$^3P_0^o$	1007672	992968
23	$4s^24p4d^*$	3	$^3D_3^o$	1015349	1001508
24	$4s^24p^*4d^*$	1	$^3D_1^o$	1029393	
25	$4s^24p^*4d$	2	$^3D_2^o$	1046884	
26	$4s^24p4d$	3	$^1F_3^o$	1082008	1071440
27	$4s^24p4d$	1	$^1P_1^o$	1108690	1072589

TABLE 2. MCDHF Energy Levels (in cm^{-1}) of $4s^24p^2$, $4s4p^3$, and $4s^24p4d$ Configurations for Te XXI and Ba XXV

Index	*jj*-coupling	*J*	$(LS)^p$	MCDHF, cm^{-1}	
				Te XXI	Ba XXV
1	$4s^24p^{*2}$	0	$^3P_0^e$	0	0
2	$4s^24p^*4p$	1	$^3P_1^e$	87506	142288
3	$4s^24p^*4p$	2	$^3P_2^e$	106473	164496
4	$4s^24p^2$	2	$^1D_2^e$	208907	323809
5	$4s^24p^2$	0	$^1S_0^e$	255756	376144
6	$4s4p^{*2}4p$	2	$^5S_2^o$	441507	569572
7	$4s4p^{*2}4p$	1	$^3D_1^o$	513288	648998

Continue Table 2

Index	*jj*-coupling	*J*	$(LS)^{\mathrm{p}}$	MCDHF, cm^{-1}	
				Te XXI	Ba XXV
8	$4s4p^24p^*$	2	$^3D_2^o$	540065	709899
9	$4s4p^24p^*$	3	$^3D_3^o$	569415	749085
10	$4s4p^24p^*$	0	$^3P_0^o$	609588	794682
11	$4s4p^24p^*$	1	$^3P_1^o$	621766	812258
12	$4s4p^3$	2	$^3P_2^o$	628567	815334
13	$4s4p^24p^*$	1	$^3S_1^o$	671343	858737
14	$4s4p^24p^*$	2	$^1D_2^o$	707408	949299
15	$4s4p^3$	1	$^1P_1^o$	785953	1032113
16	$4s^24p^*4d^*$	2	$^3F_2^o$	731944	931958
17	$4s^24p^*4d$	3	$^3F_3^o$	781404	970150
18	$4s^24p4d^*$	2	$^3P_2^o$	810864	996989
19	$4s^24p4d^*$	1	$^3P_1^o$	813074	1000363
20	$4s^24p4d$	4	$^3F_4^o$	858164	1093024
21	$4s^24p4d$	2	$^1D_2^e$	887452	1123664
22	$4s^24p4d$□	0	$^3P_0^o$	894333	1127840
23	$4s^24p4d^*$	3	$^3D_3^o$	902735	1134929
24	$4s^24p^*4d^*$	1	$^3D_1^o$	905764	1103053
25	$4s^24p^*4d$	2	$^3D_2^o$	920588	1176572
26	$4s^24p4d$	3	$^1F_3^o$	964355	1209890
27	$4s^24p4d$	1	$^1P_1^o$	982530	1240623

The calculated MCDHF results have been compared with the theoretical results obtained by Nagy and El-Sayed [9] who used the multiconfiguration Dirac–Fock method (MCDF) to calculate energies for 32 low-lying levels as listed in Table 1. The data show that the MCDHF energy levels are in excellent agreement (within ~0.4%) with the MCDF theoretical results.

The wavelengths, transition rates, and line strengths for the $4s^24p^2$–$4s4p^3$, and $4s^24p^2$–$4s^24p4d$ allowed transitions calculated using the MCDHF method are reported in Tables 3–5. The calculated MCDHF transition rates are presented in both the length and velocity gauges. The agreement between the length and velocity forms of the transition rates is within 0–5% for all the strong transitions (i.e., for $f \geq 0.10$). The exceptions to this are the few transitions for which the agreement is observed within about 10%. This overall good agreement is satisfactory and also gives a clear indication of the result accuracy.

TABLE 3. Wavelengths, Transition Rates, and Line Strengths for Te XXI

Lower	Upper	λ, Å	A_L, s^{-1}	A_V, s^{-1}	S_L
$4s^24p^2\,{}^3P_0^e$	$4s4p^3\,{}^3D_1^o$	194.82	2.19(10)	2.24(10)	2.40(–1)
	$4s4p^3\,{}^3P_1^o$	160.83	4.75(9)	4.67(9)	2.92(–2)
	$4s4p^3\,{}^3S_1^o$	148.96	1.76(10)	1.73(10)	8.63(–2)
	$4s4p^3\,{}^1P_1^o$	127.23	4.56(9)	4.40(9)	1.39(–2)
	$4s^24p4d\,{}^3P_1^o$	122.99	2.36(11)	2.30(11)	6.50(–1)
	$4s^24p4d\,{}^3D_1^o$	110.40	6.32(8)	6.25(8)	1.26(–3)
	$4s^24p4d\,{}^1P_1^o$	101.78	1.75(9)	1.80(9)	2.72(–3)
$4s^24p^2\,{}^1S_0^e$	$4s4p^3\,{}^3D_1^o$	388.30	3.44(7)	3.58(7)	2.98(–3)
	$4s4p^3\,{}^3P_1^o$	273.22	8.46(8)	8.54(8)	2.56(–2)
	$4s4p^3\,{}^3S_1^o$	240.62	2.45(9)	2.52(9)	5.06(–2)
	$4s4p^3\,{}^3P_1^o$	188.61	1.95(10)	2.01(10)	1.94(–1)
	$4s^24p4d\,{}^3P_1^o$	179.74	3.35(9)	3.19(9)	2.88(–2)
	$4s^24p4d\,{}^3D_1^o$	154.07	7.31(8)	6.95(8)	3.96(–3)
	$4s^24p4d\,{}^3P_1^o$	137.78	2.16(11)	2.07(11)	8.35(–1)
$4s^24p^2\,{}^3P_1^e$	$4s4p^3\,{}^3P_0^o$	191.54	2.41(10)	2.45(10)	8.35(–2)
	$4s4p^3\,{}^3D_1^o$	234.86	1.29(8)	1.16(8)	2.48(–3)
	$4s4p^3\,{}^3P_1^o$	187.17	3.00(10)	3.03(10)	2.91(–1)

Continue Table 3

Lower	Upper	λ, Å	A_L, s^{-1}	A_V, s^{-1}	S_L
	$4s4p^3\,^3S_1^o$	171.28	2.98(10)	2.96(10)	2.22(–1)
	$4s4p^3\,^1P_1^o$	143.17	2.43(10)	2.38(10)	1.06(–1)
	$4s4p^3\,^5S_2^o$	282.48	1.33(9)	1.40(9)	7.38(–2)
	$4s4p^3\,^3D_2^o$	220.96	8.38(9)	8.42(9)	2.23(–1)
	$4s4p^3\,^3P_2^o$	184.82	3.00(8)	3.01(8)	4.68(–3)
	$4s4p^3\,^3D_2^o$	161.31	7.60(8)	7.44(8)	7.88(–3)
	$4s^24p4d\,^3P_0^o$	123.92	2.08(11)	1.98(11)	1.95(–1)
	$4s^24p4d\,^3P_1^o$	137.80	7.98(9)	7.91(9)	3.09(–2)
	$4s^24p4d\,^3D_1^o$	122.19	1.30(11)	1.25(11)	3.51(–1)
	$4s^24p4d\,^1P_1^o$	111.71	5.52(9)	5.50(9)	1.14(–2)
	$4s^24p4d\,^3F_2^o$	155.14	1.18(8)	1.02(8)	1.09(–3)
	$4s^24p4d\,^3P_2^o$	138.22	1.13(11)	1.08(11)	7.36(–1)
	$4s^24p4d\,^1D_2^o$	124.99	1.22(11)	1.18(11)	5.88(–1)
	$4s^24p4d\,^3D_2^o$	120.02	2.00(10)	1.93(10)	8.54(–2)
$4s^24p^2\,^3P_2^e$	$4s4p^3\,^3D_1^o$	245.81	2.65(9)	2.65(9)	5.83(–2)
	$4s4p^3\,^3P_1^o$	194.06	6.00(8)	6.12(8)	6.49(–3)
	$4s4p^3\,^3S_1^o$	177.03	8.83(10)	8.78(10)	7.26(–1)
	$4s4p^3\,^1P_1^o$	147.17	1.06(9)	9.88(8)	5.01(–3)
	$4s4p^3\,^5S_2^o$	298.48	8.23(8)	8.47(8)	5.40(–2)
	$4s4p^3\,^3D_2^o$	230.63	3.09(8)	3.15(8)	9.37(–3)
	$4s4p^3\,^3P_2^o$	191.53	3.33(10)	3.38(10)	5.77(–1)
	$4s4p^3\,^1D_2^o$	166.41	5.87(8)	5.79(8)	6.68(–3)
	$4s4p^3\,^3D_3^o$	216.01	4.91(9)	4.96(9)	1.71(–1)
	$4s^24p4d\,^3P_1^o$	141.62	7.23(9)	7.12(9)	3.04(–2)
	$4s^24p4d\,^3D_1^o$	125.19	3.98(10)	3.87(10)	1.15(–1)
	$4s^24p4d\,^1P_1^o$	114.21	3.39(7)	3.18(7)	7.49(–5)
	$4s^24p4d\,^3F_2^o$	160.00	1.03(10)	9.95(9)	1.04(–1)
	$4s^24p4d\,^3P_2^o$	142.06	7.02(10)	6.98(10)	4.96(–1)
	$4s^24p4d\,^1D_2^o$	128.12	1.23(11)	1.21(11)	6.39(–1)
	$4s^24p4d\,^3D_2^o$	122.91	2.42(10)	2.40(10)	1.11(–1)
	$4s^24p4d\,^3F_3^o$	148.27	2.92(10)	2.89(10)	3.29(–1)
	$4s^24p4d\,^3D_3^o$	125.66	2.49(11)	2.45(11)	1.70(0)
	$4s^24p4d\,^1F_3^o$	116.63	4.98(10)	4.96(10)	2.73(–1)
$4s^24p^2\,^1D_2^e$	$4s4p^3\,^3D_1^o$	328.53	2.77(8)	2.80(8)	1.45(–2)
	$4s4p^3\,^3P_1^o$	242.21	2.38(8)	2.21(8)	5.22(–3)
	$4s4p^3\,^3S_1^o$	216.25	2.54(9)	2.60(9)	3.80(–2)
	$4s4p^3\,^1P_1^o$	173.30	8.74(10)	8.71(10)	6.74(–1)
	$4s4p^3\,^5S_2^o$	429.92	2.56(7)	2.64(7)	5.02(–3)
	$4s4p^3\,^3D_2^o$	301.97	1.99(8)	2.03(8)	1.35(–2)
	$4s4p^3\,^3P_2^o$	238.29	1.89(9)	1.89(9)	6.33(–2)
	$4s4p^3\,^1D_2^o$	200.60	2.27(10)	2.30(10)	4.52(–1)
	$4s4p^3\,^3D_3^o$	277.39	2.85(9)	2.95(9)	2.10(–1)
	$4s^24p4d\,^3P_1^o$	165.70	4.72(9)	4.55(9)	3.18(–2)
	$4s^24p4d\,^3D_1^o$	143.63	6.46(10)	6.39(10)	2.83(–1)
	$4s^24p4d\,^1P_1^o$	129.37	4.05(8)	4.25(8)	1.29(–3)
	$4s^24p4d\,^3F_2^o$	191.43	2.36(9)	2.42(9)	4.08(–2)
	$4s^24p4d\,^3P_2^o$	166.31	6.90(9)	6.76(9)	7.83(–1)
	$4s^24p4d\,^1D_2^o$	147.52	1.67(10)	1.58(10)	1.33(–1)
	$4s^24p4d\,^3D_2^o$	140.64	1.73(11)	1.65(11)	1.19(0)
	$4s^24p4d\,^3F_3^o$	174.87	3.09(8)	2.81(8)	5.71(–3)
	$4s^24p4d\,^3D_3^o$	144.26	2.65(10)	2.54(10)	2.75(–1)
	$4s^24p4d\,^1F_3^o$	132.49	2.48(11)	2.46(11)	1.99(0)

TABLE 4. Wavelengths, Transition Rates, and Line Strengths for Xe XXIII

Lower	Upper	λ, Å	A_L, s^{-1}	A_V, s^{-1}	S_L
$4s^24p^2\,^3P_0^e$	$4s4p^3\,^3D_1^o$	172.86	2.94(10)	2.99(10)	2.24(–1)
	$4s4p^3\,^3P_1^o$	140.45	6.25(9)	6.23(9)	2.58(–2)
	$4s4p^3\,^3S_1^o$	131.55	2.12(10)	2.09(10)	7.10(–2)
	$4s4p^3\,^1P_1^o$	111.09	4.21(10)	4.16(10)	8.65(–2)
	$4s^24p4d\,^3P_1^o$	111.33	2.92(11)	2.95(11)	5.81(–1)
	$4s^24p4d\,^3D_1^o$	97.14	6.16(8)	6.09(8)	8.37(–4)
	$4s^24p4d\,^1P_1^o$	90.20	1.93(9)	1.90(9)	2.09(–3)
$4s^24p^2\,^1S_0^e$	$4s4p^3\,^3D_1^o$	374.06	3.24(7)	3.29(7)	2.51(–3)
	$4s4p^3\,^3P_1^o$	249.48	1.14(9)	1.17(9)	2.61(–2)
	$4s4p^3\,^3S_1^o$	222.72	2.98(9)	3.02(9)	4.89(–2)
	$4s4p^3\,^1P_1^o$	169.78	2.12(10)	2.16(10)	1.53(–1)
	$4s^24p4d\,^3P_1^o$	168.19	1.26(9)	1.32(9)	8.96(–3)
	$4s^24p4d\,^3D_1^o$	139.36	1.13(9)	1.10(9)	4.53(–3)
	$4s^24p4d\,^1P_1^o$	125.49	2.78(11)	2.78(11)	8.12(–1)
$4s^24p^2\,^3P_1^e$	$4s4p^3\,^3P_0^o$	171.04	3.02(10)	3.06(10)	7.45(–2)
	$4s4p^3\,^3D_1^o$	214.59	3.68(8)	3.59(8)	5.38(–3)
	$4s4p^3\,^3P_1^o$	166.81	4.00(10)	4.03(10)	2.75(–1)
	$4s4p^3\,^3S_1^o$	154.40	3.28(10)	3.27(10)	1.79(–1)
	$4s4p^3\,^1P_1^o$	126.96	1.53(10)	1.49(10)	4.56(–2)
	$4s4p^3\,^5S_2^o$	256.06	1.98(9)	2.10(9)	8.21(–2)
	$4s4p^3\,^3D_2^o$	197.06	9.54(9)	9.68(9)	1.80(–1)
	$4s4p^3\,^3P_2^o$	165.27	5.94(8)	5.95(8)	6.61(–3)
	$4s4p^3\,^1D_2^o$	142.93	1.19(8)	1.17(8)	8.59(–4)
	$4s^24p4d\,^3P_0^o$	111.68	2.64(11)	2.67(11)	1.82(–1)
	$4s^24p4d\,^3P_1^o$	125.92	3.52(10)	3.53(10)	1.04(–1)
	$4s^24p4d\,^3D_1^o$	109.03	8.67(10)	8.74(10)	1.66(–1)
	$4s^24p4d\,^1P_1^o$	100.36	6.37(9)	6.41(9)	9.53(–3)
	$4s^24p4d\,^3F_2^o$	138.61	5.95(9)	5.86(9)	3.90(–2)
	$4s^24p4d\,^3P_2^o$	124.97	1.06(11)	1.06(11)	5.09(–1)
	$4s^24p4d\,^1D_2^o$	114.07	1.49(11)	1.51(11)	5.20(–1)
	$4s^24p4d\,^3D_2^o$	106.99	1.27(10)	1.27(10)	3.84(–2)
$4s^24p^2\,^3P_2^e$	$4s4p^3\,^3D_1^o$	224.52	4.03(9)	4.04(9)	6.76(–2)
	$4s4p^3\,^3P_1^o$	172.74	5.66(8)	5.68(8)	4.32(–3)
	$4s4p^3\,^3S_1^o$	159.48	1.04(11)	1.04(11)	6.24(–1)
	$4s4p^3\,^1P_1^o$	130.37	3.57(9)	3.43(9)	1.17(–2)
	$4s4p^3\,^5S_2^o$	270.33	1.22(9)	1.28(9)	5.96(–2)
	$4s4p^3\,^3D_2^o$	197.40	3.73(8)	3.79(8)	7.97(–3)
	$4s4p^3\,^3P_2^o$	171.09	4.03(10)	4.08(10)	4.98(–1)
	$4s4p^3\,^1D_2^o$	147.27	2.24(9)	2.24(9)	1.76(–2)
	$4s4p^3\,^3D_3^o$	191.86	5.82(9)	5.98(9)	1.42(–1)
	$4s^24p4d$	129.36	1.61(10)	1.48(10)	5.18(–2)
	$4s^24p4d\,^3D_1^o$	111.61	4.18(10)	4.23(10)	8.40(–2)
	$4s^24p4d\,^3P_1^o$	142.79	3.79(10)	3.90(10)	2.72(–1)
	$4s^24p4d\,^3F_2^o$	128.36	8.79(10)	8.82(10)	4.59(–1)
	$4s^24p4d\,^3P_2^o$	114.79	2.05(11)	2.09(11)	7.64(–1)
	$4s^24p4d\,^1D_2^o$	109.47	7.68(9)	7.53(9)	2.48(–2)
	$4s^24p4d\,^3D_2^o$	135.24	4.14(10)	4.15(10)	3.54(–1)
	$4s^24p4d\,^3D_3^o$	114.38	3.06(11)	3.08(11)	1.54(0)
	$4s^24p4d\,^1F_3^o$	105.42	4.52(10)	4.49(10)	1.83(–1)
$4s^24p^2\,^1D_2^e$	$4s4p^3\,^3D_1^o$	315.51	2.57(8)	2.59(8)	1.20(–2)
	$4s4p^3\,^3P_1^o$	222.01	5.92(8)	5.84(8)	9.59(–3)
	$4s4p^3\,^3S_1^o$	200.57	3.22(9)	3.32(9)	3.85(–2)

Continue Table 4

Lower	Upper	λ, Å	A_L, s^{-1}	A_V, s^{-1}	S_L
	$4s4p^3\,{}^1P_1^o$	156.60	8.57(10)	8.52(10)	4.87(–1)
	$4s4p^3\,{}^5S_2^o$	414.14	2.54(7)	2.70(7)	4.46(–3)
	$4s4p^3\,{}^3D_2^o$	279.03	2.76(8)	2.86(8)	1.48(–2)
	$4s4p^3\,{}^3P_2^o$	219.29	2.75(9)	2.76(9)	7.16(–2)
	$4s4p^3\,{}^1D_2^o$	181.63	1.40(10)	1.43(10)	2.07(–1)
	$4s4p^3\,{}^3D_3^o$	254.61	3.46(9)	3.49(9)	1.97(–1)
	$4s^24p4d\,{}^3D_1^o$	130.29	1.45(11)	1.44(11)	4.77(–1)
	$4s^24p4d\,{}^1P_1^o$	118.09	9.87(9)	1.02(10)	2.83(–2)
	$4s^24p4d\,{}^3F_2^o$	174.88	1.31(9)	1.40(9)	1.73(–2)
	$4s^24p4d\,{}^3P_2^o$	153.72	1.43(10)	1.48(10)	1.29(–1)
	$4s^24p4d\,{}^1D_2^o$	134.65	1.02(10)	1.12(10)	6.12(–2)
	$4s^24p4d\,{}^3D_2^o$	127.39	2.53(11)	2.60(11)	1.29(0)
	$4s^24p4d\,{}^3F_3^o$	163.69	5.98(8)	6.16(8)	8.99(–3)
	$4s^24p4d\,{}^3D_3^o$	132.72	2.52(10)	2.61(10)	2.04(–1)
	$4s^24p4d\,{}^1F_3^o$	121.94	2.90(11)	2.90(11)	1.82(0)

TABLE 5. Wavelengths, Transition rates, and Line Strengths for Ba XXV

Lower	Upper	λ, Å	A_L, s^{-1}	A_V, s^{-1}	S_L
$4s^24p^2\,{}^3P_0^e$	$4s4p^3\,{}^3D_1^o$	154.08	3.88(10)	3.90(10)	2.10(–1)
	$4s4p^3\,{}^3P_1^o$	123.11	8.87(9)	8.79(9)	2.45(–2)
	$4s4p^3\,{}^3S_1^o$	116.45	2.61(10)	2.57(10)	6.10(–2)
	$4s4p^3\,{}^1P_1^o$	96.89	8.03(9)	8.02(9)	1.08(–2)
	$4s^24p4d\,{}^3P_1^o$	99.96	3.14(11)	3.18(11)	4.64(–1)
	$4s^24p4d\,{}^3D_1^o$	90.66	6.84(8)	6.86(8)	7.55(–4)
	$4s^24p4d\,{}^1P_1^o$	80.60	1.94(9)	1.89(9)	1.51(–3)
$4s^24p^2\,{}^1S_0^e$	$4s4p^3\,{}^3D_1^o$	366.50	2.82(7)	2.86(7)	2.06(–3)
	$4s4p^3\,{}^3P_1^o$	229.30	1.47(9)	1.51(9)	2.62(–2)
	$4s4p^3\,{}^3S_1^o$	207.21	3.45(9)	3.51(9)	4.55(–2)
	$4s4p^3\,{}^1P_1^o$	152.45	2.24(10)	2.29(10)	1.17(–1)
	$4s^24p4d\,{}^3P_1^o$	160.35	1.21(9)	1.25(9)	7.36(–3)
	$4s^24p4d\,{}^3D_1^o$	137.68	8.22(9)	8.38(9)	3.18(–2)
	$4s^24p4d\,{}^1P_1^o$	115.76	3.17(11)	3.20(11)	7.28(–1)
$4s^24p^2\,{}^3P_1^e$	$4s4p^3\,{}^3P_0^o$	153.28	3.77(10)	3.80(10)	6.69(–2)
	$4s4p^3\,{}^3D_1^o$	197.35	7.37(8)	7.25(8)	8.39(–3)
	$4s4p^3\,{}^3P_1^o$	149.26	5.25(10)	5.30(10)	2.59(–1)
	$4s4p^3\,{}^3S_1^o$	139.58	3.56(10)	3.55(10)	1.43(–1)
	$4s4p^3\,{}^1P_1^o$	112.38	7.25(10)	7.19(10)	1.52(–1)
	$4s4p^3\,{}^5S_2^o$	234.04	2.75(9)	2.81(9)	8.71(–2)
	$4s4p^3\,{}^3D_2^o$	176.18	1.07(10)	1.11(10)	1.44(–1)
	$4s4p^3\,{}^3P_2^o$	148.58	9.93(8)	1.00(9)	8.04(–3)
	$4s4p^3\,{}^1D_2^o$	123.91	9.11(9)	8.94(9)	4.27(–2)
	$4s^24p4d\,{}^3P_0^o$	101.43	3.10(11)	3.15(11)	1.60(–1)
	$4s^24p4d\,{}^3P_1^o$	116.50	5.63(10)	5.70(10)	1.32(–1)
	$4s^24p4d\,{}^3D_1^o$	104.05	2.38(11)	2.40(11)	3.98(–1)
	$4s^24p4d\,{}^1P_1^o$	910.21	7.62(9)	7.73(9)	8.50(–3)
	$4s^24p4d\,{}^3F_2^o$	126.59	1.22(10)	1.22(10)	6.10(–2)
	$4s^24p4d\,{}^3P_2^o$	116.96	1.46(11)	1.50(11)	5.78(–1)
	$4s^24p4d\,{}^1D_2^o$	101.87	1.74(11)	1.76(11)	4.54(–1)
	$4s^24p4d\,{}^3D_2^o$	96.66	1.20(10)	1.21(10)	2.68(–2)
$4s^24p^2\,{}^3P_2^e$	$4s4p^3\,{}^3D_1^o$	206.40	5.78(9)	5.81(9)	7.52(–2)
	$4s4p^3\,{}^3P_1^o$	154.38	5.03(8)	5.07(8)	2.74(–3)
	$4s4p^3\,{}^3S_1^o$	144.04	1.22(11)	1.22(11)	5.39(–1)

Continue Table 5

Lower	Upper	λ, Å	A_L, s^{-1}	A_V, s^{-1}	S_L
	$4s4p^{3\ 1}P_1^o$	115.26	1.34(9)	1.29(9)	3.04(–3)
	$4s4p^{3\ 5}S_2^o$	246.87	1.72(9)	1.80(9)	6.38(–2)
	$4s4p^{3\ 3}D_2^o$	183.35	4.13(8)	4.19(8)	6.28(–3)
	$4s4p^{3\ 3}P_2^o$	153.65	4.60(10)	4.66(10)	4.12(–1)
	$4s4p^{3\ 1}D_2^o$	127.42	1.18(10)	1.16(10)	6.03(–2)
	$4s4p^{3\ 3}D_3^o$	171.06	6.78(9)	6.86(9)	1.17(–1)
	$4s^24p4d\ ^3D_1^o$	119.67	2.77(10)	2.66(10)	7.05(–2)
	$4s^24p4d\ ^1P_1^o$	106.58	1.69(10)	1.64(10)	3.04(–2)
	$4s^24p4d\ ^3F_2^o$	130.34	5.31(7)	5.37(7)	2.90(–1)
	$4s^24p4d\ ^3P_2^o$	120.16	6.18(10)	6.27(10)	2.65(–1)
	$4s^24p4d\ ^1D_2^o$	104.29	2.43(11)	2.50(11)	6.79(–1)
	$4s^24p4d\ ^3D_2^o$	98.83	5.39(9)	5.24(9)	1.29(–2)
	$4s^24p4d\ ^3F_3^o$	124.16	5.67(10)	5.71(10)	3.75(–1)
	$4s^24p4d\ ^3D_3^o$	103.07	3.53(11)	3.56(11)	1.33(0)
	$4s^24p4d\ ^1F_3^o$	95.68	4.55(10)	4.52(10)	1.38(–1)
$4s^24p^{2\ 1}D_2^e$	$4s4p^{3\ 3}D_1^o$	307.51	2.24(8)	2.25(8)	9.66(–3)
	$4s4p^{3\ 3}P_1^o$	204.73	1.13(9)	1.08(9)	1.44(–2)
	$4s4p^{3\ 3}S_1^o$	186.94	3.89(9)	4.01(9)	3.76(–2)
	$4s4p^{3\ 1}P_1^o$	141.18	1.19(11)	1.18(11)	4.94(–1)
	$4s4p^{3\ 5}S_2^o$	406.90	2.29(7)	2.31(7)	3.81(–3)
	$4s4p^{3\ 3}D_2^o$	259.01	3.71(8)	3.77(8)	1.59(–2)
	$4s4p^{3\ 3}P_2^o$	203.45	3.55(9)	3.58(9)	7.38(–2)
	$4s4p^{3\ 1}D_2^o$	159.87	3.49(10)	3.54(10)	3.51(–1)
	$4s4p^{3\ 3}D_3^o$	235.14	4.09(9)	4.14(9)	1.84(–1)
	$4s^24p4d\ ^3D_1^o$	128.38	6.35(10)	6.31(10)	1.96(–1)
	$4s^24p4d\ ^3F_2^o$	164.51	3.12(9)	3.16(9)	3.43(–2)
	$4s^24p4d\ ^1D_2^o$	125.07	7.66(9)	7.76(9)	3.77(–2)
	$4s^24p4d\ ^3D_2^o$	117.30	2.94(11)	3.07(11)	1.17(0)
	$4s^24p4d\ ^3F_3^o$	154.78	9.43(8)	9.59(8)	1.16(–2)
	$4s^24p4d\ ^3D_3^o$	123.33	2.34(10)	2.38(10)	1.52(–1)
	$4s^24p4d\ ^1F_3^o$	112.89	3.28(11)	3.30(11)	1.63(0)

TABLE 6. Comparison between MCDHF (Å), Experiment [12, 13], and Theoretical Wavelengths (Å) of Xe XXIII Ion

Transition	Theory		Experiment	
	MCDHF	HULLAC [13]	BerlinEBIT [13]	TFR [12]
$4s^24p^{2\ 3}P_0^e – 4s^24p4d\ ^3P_1^o$	111.325	109.66	112.38	112.40
$4s^24p^2\ ^3P_1^e – 4s^24p4d\ ^1D_2^o$	114.068	110.90	114.32	
$4s^24p^{2\ 3}P_2^e – 4s^24p4d\ ^3D_3^o$	114.383	111.54	114.725	114.84
$4s^24p^2\ ^3P_2^e – 4s4p^3\ ^3S_1^o$	159.477	151.34	159.93	159.93
$4s^24p^2\ ^3P_2^e – 4s4p^{3\ 3}P_2^o$	171.091	166.73	171.42	
$4s^24p^2\ ^3P_0^e – 4s4p^{33\ 3}D_1^o$	172.860	168.92	173.003	173.23
$4s^24p^{2\ 3}P_2^e – 4s4p^{3\ 3}D_3^o$	191.856	188.33	191.461	
$4s^24p^2\ ^3P_2^e – 4s4p^{3\ 3}D_2^o$	197.404	193.93	196.795	

Table 6 shows a comparison between the MCDHF and experimental wavelengths [12, 13] and other theoretical results [13] for the Ge-like Xe ions. The comparison shows that the MCDHF wavelengths are in excellent agreement with the available experimental [12, 13] results, the difference being 0.08–1.00% for most cases. For the Xe XXIII ion, the agreement is within about 2.5% with HULLAC [13]. However, a more detailed comparison of the calculated and experimental wavelengths for these transitions indicates that the results given by our GRASP2 K calculations are in better agreement with the experimental energies than the HULLAC results of Biedermann et al. [13]. Specifically, the maximum difference between the results of the experiment and our GRASP2 K transition wavelengths is 0.939%, but the maximum difference for the HULLAC results of Biedermann et al. [13] and the experimental results is 2.992%.

Conclusion. The energy levels, wavelengths, transition rates, and line strengths have been calculated for the allowed electric dipole (E1) $4s^24p^2$–$4s4p^3$ and $4s24p^2$–$4s^24p4d$ transitions for the Ge-like ions from $Z = 52$ to 56. The calculations were performed using the multiconfiguration Dirac–Hartree–Fock (MCDHF) method, taking into account the correlations (i.e., for CV, VV) within the $n = 6$ complex and the quantum electrodynamic effects. A comparison between MCDHF results of energy levels and wavelengths with the available experimental and other theoretical results shows excellent agreement. Hopefully, the present results will help the line identification in future experimental work.

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REFERENCES

1. J. D. Gilaspy, *J. Phys. B: At. Mol. Opt. Phys.*, **34**, R93 (2001).
2. D. A. Liedahl, *Spectroscopic Challenges of Photoionized Plasmas*, Eds. G. Ferland, D. W. Savin, San Francisco, ASP Conference Series, p. 417 (2001).
3. I. M. Savukov, W. R. Johnson, *Phys. Rev. A*, **65**, 042503 (2002).
4. K. T. Cheng, R. A. Wagner, *Phys. Rev. A*, **36**, 5435–5438 (1987).
5. S. A. Blundell, W. R. Johnson, J. Sapirstein, *Phys. Rev. A*, **43**, 3407–3418 (1991).
6. E. Biémont, A. El Himdy, H. P. Garnir, *J. Quant. Spectrosc. Radiat. Transfer*, **43**, 437–443 (1990).
7. U. Litzén, X. Zeng, *J. Phys. B: At. Mol. Opt. Phys.*, **24**, L45 (1991).
8. J.-G. Li, E. Träbert, C.-Z. Dong, *Phys. Scr.*, **83**, 015301 (2011).
9. O. Nagy, F. El-Sayed, *At. Data Nucl. Data Tables*, **98**, 373–390 (2012).
10. P. Palmeri, P. Quinet, E. Biémont, E. Trabert, *At. Data Nucl. Data Tables*, **93**, 355–374 (2007).
11. U. Litzén, J. Reader, *Phys. Scr.*, **39**, 468–473 (2006).
12. C. Breton, C. DeMichelis, W. Hecq, M. Mattioli, J. Ramette, B. Saoutic, C. Bauche-Arnoult, J. Bauche, J. F. Wyart, *Phys. Scr.*, **37**, 33–37 (1988).
13. C. Biedermann, R. Radtke, G. Fußann, J. L. Schwob, P. Mandelbaum, *Nucl. Instrum. Methods Phys. Res. B*, **235**, 126–130 (2005).
14. E. Träbert, *Phys. Scr.*, **T144**, 014004 (2011) .
15. C. Suzuki, T. Kato, H.A. Sakaue, D. Kato, K. Sato, N. Tamura, S. Sudo, N. Yamamoto, H. Tanuma, H. Ohashi, R. D'Arcy, G. O'Sullivan, *J. Phys. B: At. Mol. Opt. Phys.*, **43**, 074027 (2010).
16. J. P. Desclau, P. Indelicato, *MCDFGME, a MultiConfiguration Dirac-Fock and General Matrix Elements Program, Release 2005*; http://dirac.spectro.jussieu.fr/mcdf.
17. F. Parpia, C. Froese Fischer, I. P. Grant, *Comput. Phys. Commun.*, **94**, 249–271 (1996).
18. J. Olsen, M. Godefroid, P. Jönsson, P. A. Malmquist, C. Froese Fischer, *Phys. Rev. E*, **52**, 4499–4508 (1995).