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Electric Quadrupole (E2) and Magnetic Dipole (M1) Transitions for Doubly and Triply Ionized Krypton, Xenon, and Radon

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Abstract: We have reported the wavelengths, transition probabilities (or rates), oscillator strengths and line strengths for forbidden transitions (electric quadrupole, E2, and magnetic dipole, M1) in doubly and triply ionized krypton, xenon and radon using the general-purpose relativistic atomic structure package (GRASP). The results obtained from transitions between the levels of ground state configuration are in agreement with other available results in literature. The data on forbidden transitions between high levels for these ions have been firstly presented in this work.

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1. Introduction

The atomic data of forbidden transitions have great importance in the understanding of astronomical spectra; because of transitions from metastable levels occur at much longer wavelengths than other transitions in the same ion for charged ions [1,2]. Using various theories, the rates of the optical allowed transitions can be calculated accurately. But weak forbidden transitions are affected by many factors such as electron correlation, relativistic effects including the Breit interaction [3]. Due to importance of inert gases in fields such as laser physics, astrophysics etc., their atomic data are much significant [4].

The doubly ionized krypton (Kr III, $Z=36$), xenon (Xe III, $Z=54$) and radon (Rn III, $Z=86$) atoms are isoelectronic with neutral selenium, tellurium and polonium, respectively. These ions have ns^2np^4 electron ground configuration ($n=4, 5$, and 6 , for Kr III, Xe III, and Rn III, respectively). The ground level for ions is $np^4\ ^3P_2$, and this level is followed by 3P_1 , 3P_0 , 1D_2 and 1S_0 in the same configuration. The triply ionized krypton (Kr IV), xenon (Xe IV) and radon (Rn IV) belongs to the arsenic, antimony and bismuth isoelectronic sequence, respectively. These ions have ns^2np^3 ground state configuration ($n=4, 5$ and 6 , respectively). $ns^2np^3\ ^4S_{3/2}$ is the ground level and this level is followed by $^2D^{\circ}_{3/2}$, $^2D^{\circ}_{5/2}$, $^2P^{\circ}_{1/2}$ and $^2P^{\circ}_{3/2}$ in the same configuration. Because of krypton and xenon have extensive emission spectrum, these atoms and their ions are particularly interesting for production of light sources, lamps and development of lasers and laser techniques [5]. Radon is a radioactive noble gas element, which is used in medicine [6]. Garstang reported calculations of the transition probabilities of forbidden lines for some ions [7]. Using the HFR method, Biémont and Hansen calculated energy levels and radiative transition probabilities in the ground configurations of the sulfur and selenium isoelectronic sequences up to molybdenum and silver, respectively [8]. Sterling presented multi-configuration Breit-Pauli distorted-wave photoionization (PI) cross sections, radiative recombination (RR) and dielectronic recombination (DR) rate coefficients for the first six krypton ions, using the AUTOSTRUCTURE code [9]. Transition probabilities were given of forbidden lines for some atoms and ions by Osterbrock [10]. Calamai and Johnson measured radiative lifetimes of several metastable states of doubly and triply ionized Ar, Kr, and Xe [11]. Using the HFR method, Biémont et al. obtained the energy levels and radiative transition probabilities for states within the $5p^k$ ($k=1-5$) configurations of atoms and ions [12]. Hansen and Persson revised analysis of the $5p^4$ ground configuration of

two-times ionized xenon and reevaluated of transition probabilities for forbidden lines within this configuration [13]. Humphreys presented the third spectrum of krypton [14]. For Rn III and Rn IV, only Biémont and Quinet presented a study about forbidden transition parameters [15]. Also we reported electric dipole (E1) transition parameters, energies and lifetimes for these ions [16-18].

The aim of this work, the forbidden transition parameters such as wavelengths, transition rates (or probabilities), oscillator strengths and line strengths of doubly and triply ionized Kr, Xe and Rn have been presented for electric quadrupole (E2) and magnetic dipole (M1) transitions between the energy levels which have the same parity. Calculations have been made using the GRASP atomic structure package based on a fully relativistic MCDF method. Breit interactions (magnetic interaction between the electrons and retardation effects of the electron-electron interaction) for relativistic effects, quantum electrodynamical (QED) contributions (self-energy and vacuum polarization) and correlation effects (valence-valence (VV), core-valence (CV) and core-core (CC)) which are important for electronic structure and spectroscopic properties of many electron systems, are included by MCDF method. In calculations various configuration sets have been considered for correlation effects (including VV, CV and CC correlations). But the best results have been obtained according to CC correlations for six ions. In table 1, CC configuration sets have been given.

Table 1. Configuration sets taken in calculations for doubly and triply ionized krypton, xenon and radon.

Kr III	4s ² 4p ⁴ , 4s4p ⁵ , 4p ⁶ , 4s ² 4p ³ 5s, 4p ⁵ 5s, 4s ² 4p ³ 6s, 4s ² 4p ³ 5p
Xe III	5s ² 5p ⁴ , 5p ⁶ , 5s5p ⁴ 5d, 5s ² 5p ² 5d ² , 5p ⁴ 5d ² , 5s5p ⁵ , 5s ² 5p ³ 5d, 5p ⁵ 5d, 5s ² 5p ³ 6s, 5s ² 5p ³ 6p, 5s ² 5p ³ 6d, 5s5p ³ 6s ² , 5s5p ³ 7s ² , 5p ⁴ 6s ² , 5p ⁵ 6s, 5s ² 5p ³ 4f
Rn III	6s ² 6p ⁴ , 6s ² 6p ³ 7s, 6s ² 6p ³ 7p, 6s ² 6p ³ 6d, 6s ² 6p ² 6d7s, 6s ² 6p ² 7s ² , 6s ² 6p ³ 7d, 6s6p ⁵ , 6s6p ³ 7s ² , 6s6p ³ 8s ² , 6s ² 6p ³ 8s, 6p ⁶ , 6p ⁴ 6d ² , 6p ⁵ 6d, 6p ⁴ 7s ² , 6p ⁵ 7s, 6p ⁴ 6d7s
Kr IV	4s ² 4p ³ , 4s ² 4p ² 5p, 4s ² 4p ² 6s, 4s ² 4p5s ² , 4s ² 4p ² 5s, 4s ² 5d ³ , 4s ² 4p ² 5d, 4s ² 4p5p ² , 4s ² 5p ³ , 4s4p ⁴ , 4s ² 4p4f ² , 4s ² 4p ² 4f, 4p ⁵
Xe IV	4d ¹⁰ 5s ² 5p ³ , 4d ¹⁰ 5s5p ⁴ , 4d ¹⁰ 5s ² 5p ² 5d, 4d ¹⁰ 5s ² 5p ² 6s, 4d ¹⁰ 5s ² 5p ² 4f, 4d ¹⁰ 5s ² 5p ² 6p, 4d ¹⁰ 5p ⁵ , 4d ¹⁰ 5s ² 5p5d ² , 4d ¹⁰ 5s5p ² 6s ² , 4d ¹⁰ 5p ³ 4f ² , 4d ¹⁰ 5d ⁵ , 4d ⁹ 5s ² 5p ⁴ , 4d ⁷ 5s ² 5p ⁶ , 4d ⁹ 5s5p ⁵
Rn IV	6s ² 6p ³ , 6s ² 6p ² 7s, 6s ² 6p ² 7p, 6s ² 6p ² 6d, 6s ² 6p6d7s, 6s ² 6p7s ² , 6s ² 6p ² 7d, 6s ² 6p ² 8s, 6s6p ⁴ , 6s6p ² 7s ² , 6s6p ² 8s ² , 6p ⁵ , 6p ³ 6d ² , 6p ⁴ 6d, 6p ³ 7s ² , 6p ⁴ 7s, 6p ³ 6d7s, 6s ² 6p ² 5f

2. Computational Details

The general-purpose relativistic atomic structure package, GRASP code [19] is based on a fully relativistic multiconfiguration Dirac-Fock (MCDF) method [20], and uses Thomas-Fermi and Coulomb potential for calculate wavefunctions according to JJ and LS coupling. In the MCDF method [20] an atomic state can be expanded as a linear combination of configuration state functions (CSFs)

$$\Psi_a(PJM) = \sum_{r=1}^{n_c} C_r(\alpha) |\gamma_r(PJM)\rangle, \quad (1)$$

where n_c is the number of CSFs included in the evaluation of atomic state functions and C_r is the mixing coefficient; and is optimized usually on the basis of the many-electron Dirac-Coulomb Hamiltonian. This method is basic and requires no knowledge of the internal coupling of the CSFs with a given parity P and angular momentum (J, M) . The CSFs are the sum of products of single-electron Dirac spinors,

$$\phi(r, \theta, \varphi, \sigma) = \frac{1}{r} \begin{pmatrix} P(r) \chi_{\kappa m}(\theta, \varphi, \sigma) \\ iQ(r) \chi_{-\kappa m}(\theta, \varphi, \sigma) \end{pmatrix}, \quad (2)$$

where κ is a quantum number and $\chi_{\kappa m}$ is the spinor spherical harmonic in the LSJ coupling scheme and $P(r)$ and $Q(r)$ are large and small radial components of one-electron wavefunctions represented on a logarithmic grid. The energy functional is based on the Dirac-Coulomb Hamiltonian in form

$$H_{DC} = \sum_{j=1}^N [C\alpha_j \cdot \mathbf{p}_j + (\beta_j - 1)c^2 + V(r_j)] + \sum_{j < k}^N \frac{1}{r_{jk}}, \quad (3)$$

where $V(r_j)$ is the electron-nucleon interaction. Once initial and final state functions have been calculated, the radiative matrix element for radiative properties computation can be obtained from

$$O_{if} = \langle \psi(i) | \mathbf{O}_q^{\pi(k)} | \psi(f) \rangle, \quad (4)$$

where $\mathbf{O}_q^{\pi(k)}$ is a spherical operator of rank k and parity π , and $\pi(\kappa)$ is $\pi = (-1)^k$, for an electric multipole transition or $\pi = (-1)^{k+1}$, for a magnetic multipole transition. The largest transition probability is for electric dipole (E1) radiation, dominated by the least factor $1/\alpha^2$ over other types of transitions (E2, M1, M2, etc.).

For a transition $i \rightarrow j$, the absorption oscillator strength (f_{ij}) and transition probabilities (A_{ji} , in s^{-1}) are related by the following expression:

$$f_{ij} = \frac{mc}{8\pi^2 e^2} \lambda_{ji}^2 \frac{\omega_j}{\omega_i} A_{ji} = 1.49 \times 10^{-16} \lambda_{ji}^2 (\omega_j / \omega_i) A_{ji} , \quad (5)$$

Where m and e are the electron mass and charge, respectively, c is the velocity of light, λ_{ji} is the transition energy/wavelength in Å, and ω_i and ω_j are the statistical weights of the lower i and upper j levels, respectively. Similarly, the oscillator strength f_{ij} (dimensionless) and the line strength S (in a.u) are related by

$$A_{ji} = \frac{1.1199 \times 10^{18}}{\omega_j \lambda_{ji}^5} S^{E2} \quad \text{and} \quad f_{ij} = \frac{167.89}{\lambda_{ji}^3 \omega_i} S^{E2} , \quad (6)$$

for the electric quadrupole transitions, and

$$A_{ji} = \frac{2.6974 \times 10^{13}}{\omega_j \lambda_{ji}^3} S^{M1} \quad \text{and} \quad f_{ij} = \frac{4.044 \times 10^{-3}}{\lambda_{ji} \omega_i} S^{M1} . \quad (7)$$

for the magnetic dipole transitions [21]. In calculations, we have used the option *extended average level* (EAL) averaging of the expression energy. It is extended to configuration states with not only different total angular momenta but also with different parities. Also, Breit corrections (magnetic interaction between the electrons and retardation effects of the electron-electron interaction), and QED (self-energy and vacuum polarization), and various correlation contributions have been considered. Because of the Coulomb interaction between the electrons, the electron correlation effects are also important, in particular, on fine structure and transitions. Therefore, the configurations including excitations from valence and core have been taken into account. QED contributions are self-energy and vacuum polarization, which are also included in the computations of the transition energy. The finite-nucleus effect is taken into account by assuming an extended Fermi distribution for the nucleus. Both the Breit and QED contributions are treated as perturbation and are not included directly in the self-consistent field procedure. The mixing coefficients are calculated by diagonalizing the modified Hamiltonian.

3. Results and Discussion

In this work, by employing the MCDF method [20], we have presented the forbidden transition (E2 and M1) parameters such as wavelengths, transition probabilities, A_{ji} (in s^{-1}), oscillator strengths, f_{ij} , and line strengths, S_{ij} (in a. u.) between the levels which have the same parities for doubly and triply ionized krypton, xenon and radon according to selected configurations in Table 1. The calculations have been done choosing *extended average level* (EAL) option for each ion in this paper. Also, the Breit corrections, QED contributions and various correlation effects have been considered. Owing to the Coulomb interaction between the electrons, the electron correlation effects are also important, in particular, on fine structure and transitions. Therefore, the configurations have been taken into account for calculations according to valence-valence, core-valence and core-core correlations. Because of the best results have been obtained according to CC correlations, only these results in here have been presented for six ions. Also we reported energies, lifetimes and electric dipole (E1) transition parameters, for these ions [16-18]. Other work values are indicated below the tables with a superscript lower case. And, only odd-parity states have been indicated by the superscript “o” in tables. Also, the number in brackets represents the power of 10 in tables. All the E2 and M1 transition values have been computed in the length form, which is considered to be more accurate than the velocity form [22]. In previous works [7-15], there is only forbidden transition probabilities and some wavelengths between the ground state levels for each ion. So we have only compared with these data. In tables 2-7 include the ratios of transition probabilities [MCDF/Other work] for comparison. At the same time, we have presented new values for forbidden transition parameters. This data is presented for the first time in this study.

3.1. E2 and M1 transitions for doubly ionized krypton, xenon and radon

We have obtained 734, 51408, and 32972 electric quadrupole transitions, and 650, 36782, and 24456 magnetic dipole transitions for Kr III, Xe III and Rn III, respectively. In Table 2, 3 and 4 have been presented the E2 and M1 transitions between the levels of ground state configuration for Kr III, Xe III and Rn III, respectively. In these tables we have only compared the transition probabilities and a few wavelength values between the ground state levels with other works [7-15] in the available literature. Except the transitions $3s^23p^4\ ^3P_2 - ^3P_0$ and $3s^23p^4\ ^3P_2 - ^1S_0$, we have found the mean ratio value 1.881 and 1.055 for E2 and M1 transitions of Kr III, respectively in

Table 2. For Xe III, this main ratio have been obtained the value 1.275 and 0.886 for E2 and M1 transitions, respectively in Table 3. In Table 4, the main ratio have been found the value 1.989 and 1.184 for E2 and M1 transitions of Rn III, respectively. There is a good agreement between obtained results and previous work results in literature, and observed values from M1 transitions are better than E2 transitions, in general. Although the transition probabilities and wavelengths for the transitions $ns^2np^4\ ^3P_2 - ^3P_0$ and $ns^2np^4\ ^3P_2 - ^1S_0$ are somewhat poor, in particular E2 transitions, the energy values of these levels reported in our previous work [18] have good agreement with comparison values ($n=4, 5$, and 6 , for Kr III, Xe III, and Rn III, respectively). For Kr III, the energies of levels from this study are 0.04666 Ry and 0.29041 Ry [18] whereas comparison values are 0.04640 Ry and 0.28620 Ry [9] for 3P_0 and 1S_0 , respectively. For Xe III, the energies are 0.07277 Ry, 0.32899 Ry [18] whereas comparison values are 0.07246 Ry and 0.32769 Ry [23] for 3P_0 and 1S_0 , respectively. And, for Rn III, obtained energy values are 0.10027 Ry, 0.67480 Ry [18] whereas comparison values are 0.10241 and 0.68130 Ry [15] for 3P_0 and 1S_0 , respectively. Therefore, we can say that the energy level values for ground state configuration of Kr III, Xe III and Rn III are good agreement with other works. However the transition parameters obtained from transitions between mentioned above levels are not in agreement with other works.

Other transition parameters such as oscillator strengths and line strengths are firstly presented here for the ground state level transitions. The first fifty transitions with the greatest transition probability (A_{ji}) have been given in Table S1, S2 and S3 for Kr III, Xe III and Rn III, respectively. And these data are new for these ions.

Table 2. The wavelengths, λ (Å), transition probabilities, A_{ji} (s^{-1}), oscillator strengths, f_{ij} , and line strengths, S_{ij} (a.u), between the ground state levels for electric quadrupole (E2) and magnetic dipole (M1) transitions in Kr III

Transitions		λ (Å)		A_{ji} (s ⁻¹)			f_{ij}	S_{ij} (a.u)
Lower Level	Upper Level	This work	Other work	This work	Other works	MCDF/Ref[8]		
E2 Transitions								
4s ² 4p ⁴ ³ P ₂	4s ² 4p ⁴ ³ P ₁	22963.00	-	6.688(-4)	7.600(-4) ^a 6.883(-4) ^b	0.971	3.172(-11)	11.439
4s ² 4p ⁴ ³ P ₂	4s ² 4p ⁴ ³ P ₀	19529.00	-	0.078(-3)	2.500(-3) ^a 2.382(-3) ^b 1.870(-3) ^c 2.010(-3) ^{c*} 2.280(-3) ^{c**}	0.033	8.953(-13)	0.199
4s ² 4p ⁴ ³ P ₂	4s ² 4p ⁴ ¹ D ₂	5715.20	6826.9 ^d	0.072	0.043 ^a 0.038 ^b	1.894	3.523(-10)	1.958
4s ² 4p ⁴ ³ P ₂	4s ² 4p ⁴ ¹ S ₀	3137.80	-	8.409	0.690 ^a 0.637 ^b 0.185 ^c 0.188 ^{c*} 0.328 ^{c**}	13.200	2.482(-9)	2.284
4s ² 4p ⁴ ³ P ₁	4s ² 4p ⁴ ¹ D ₂	7609.00	9902.2 ^d	2.857(-3)	1.000(-3) ^a 0.921(-3) ^b	3.102	4.134(-11)	0.32
4s ² 4p ⁴ ³ P ₀	4s ² 4p ⁴ ¹ D ₂	8079.80	-	9.423(-4)	3.700(-4) ^a 2.900(-4) ^b 0.167(-4) ^c 0.173(-4) ^{c*} 8.950(-4) ^{c**}	3.249	4.611(-11)	0.144
4s ² 4p ⁴ ¹ D ₂	4s ² 4p ⁴ ¹ S ₀	6958.10	-	0.789	4.500 ^a 4.121 ^b 1.240 ^c 1.240 ^{c*} 2.790 ^{c**}	0.191	1.145(-9)	11.494

Table 2 Continued

M1 Transitions								
4s ² 4p ⁴ ³ P ₂	4s ² 4p ⁴ ³ P ₁	22963.00	-	1.807	2.000 ^a	0.898	8.571(-8)	2.433
					2.012 ^b			
					1.660 ^c			
					1.760 ^{c*}			
					1.770 ^{c**}			
4s ² 4p ⁴ ³ P ₁	4s ² 4p ⁴ ³ P ₀	130590.00	-	0.023	0.023 ^a	0.793	1.971(-8)	1.909
					0.029 ^b			
					0.024 ^c			
					0.023 ^{c*}			
					0.032 ^{c**}			
4s ² 4p ⁴ ³ P ₂	4s ² 4p ⁴ ¹ D ₂	5715.20	6826.9 ^d	5.467	4.700 ^a	1.165	2.677(-8)	0.189
					4.690 ^b			
					5.030 ^c			
					5.420 ^{c*}			
					4.820 ^{c**}			
4s ² 4p ⁴ ³ P ₁	4s ² 4p ⁴ ¹ D ₂	7609.00	9902.2 ^d	0.796	0.530 ^a	1.479	1.152(-8)	0.065
					0.538 ^b			
					0.722 ^c			
					0.743 ^{c*}			
					0.671 ^{c**}			
4s ² 4p ⁴ ³ P ₁	4s ² 4p ⁴ ¹ S ₀	3634.50	3500.0 ^e	49.856	53.000 ^a	0.940	3.291(-8)	0.088
					53.020 ^b			
					45.400 ^c			
					47.200 ^{c*}			
					48.200 ^{c**}			

^a Ref. [7]; ^b Ref. [8]; ^c Ref. [9]; ^d Ref. [10]; ^e Ref. [11]

Note: c, c*, c** values are belong to the same study, which were presented different configuration sets.

Table 3. The wavelengths, λ (Å), transition probabilities, A_{ji} (s^{-1}), oscillator strengths, f_{ij} , and line strengths, S_{ij} (a.u), between the ground state levels for electric quadrupole (E2) and magnetic dipole (M1) transitions in Xe III.

Transitions		λ (Å)		A_{ji} (s ⁻¹)			f_{ij}	S_{ij} (a.u)
Lower level	Upper level	This work	Other works	This work	Other works	MCDF/Ref[13]		
E2 Transitions								
5s ² 5p ⁴ ³ P ₂	5s ² 5p ⁴ ³ P ₁	11124.0	10206.9 ^e	3.501(-2)	5.023(-2) ^a	0.508	3.897(-10)	15.970
					6.880(-2) ^b			
					6.800(-2) ^c			
5s ² 5p ⁴ ³ P ₂	5s ² 5p ⁴ ³ P ₀	12283.0		0.008(-2)	4.451(-2) ^a	0.002	3.747(-13)	0.021
					5.390(-2) ^b			
					5.200(-2) ^c			
5s ² 5p ⁴ ³ P ₂	5s ² 5p ⁴ ¹ D ₂	5495.5	5846.69 ^e	0.426	4.078 ^a	0.077	1.929(-9)	9.534
					5.520 ^b			
					0.520 ^c			
5s ² 5p ⁴ ³ P ₂	5s ² 5p ⁴ ¹ S ₀	2.722		16.310	2.770 ^a	5.845	3.625(-9)	2.179
					2.790 ^b			
					3.900 ^c			
5s ² 5p ⁴ ³ P ₁	5s ² 5p ⁴ ¹ D ₂	10861.0		2.447(-3)	0.904(-3) ^a	1.926	7.211(-11)	1.651
					1.270(-3) ^b			
					1.200(-3) ^c			
5s ² 5p ⁴ ³ P ₀	5s ² 5p ⁴ ¹ D ₂	9944.9		0.207(-3)	2.730(-3) ^a	0.055	1.533(-11)	0.089
					3.700(-3) ^b			
					3.100(-3) ^c			
5s ² 5p ⁴ ¹ D ₂	5s ² 5p ⁴ ¹ S ₀	5396.20		4.951	7.216 ^a	0.513	4.323(-9)	20.228
					9.640 ^b			
					13.00 ^c			
M1 Transitions								
5s ² 5p ⁴ ³ P ₂	5s ² 5p ⁴ ³ P ₁	11124.0	10206.9 ^e	14.790	19.170 ^a	0.799	1.646(-7)	2.264
					18.500 ^b			
					19.000 ^c			

Table 3 Continued

5s ² 5p ⁴ ³ P ₁	5s ² 5p ⁴ ³ P ₀	117910.0		1.000(-2)	5.083(-2) ^a	0.151	5.747(-8)	1.676
					6.590(-2) ^b			
					6.700(-2) ^c			
5s ² 5p ⁴ ³ P ₂	5s ² 5p ⁴ ¹ D ₂	5495.50	5846.69 ^e	20.048	21.520 ^a	0.963	9.077(-8)	0.617
					20.800 ^b			
					21.000 ^c			
5s ² 5p ⁴ ³ P ₁	5s ² 5p ⁴ ¹ D ₂	10861.0		0.961	0.630 ^a	1.567	2.535(-8)	0.228
					0.613 ^b			
					0.620 ^c			
5s ² 5p ⁴ ³ P ₁	5s ² 5p ⁴ ¹ S ₀	3605.0	3800 ^d	181.470	192.0 ^a	0.950	1.179(-7)	0.315
					191.0 ^b			
					210.0 ^c			

^a Ref. [12]; ^b Ref. [13]; ^c Ref. [7]; ^d Ref. [11]; ^e Ref. [14]

Table 4. The wavelengths, λ (Å), transition probabilities, A_{ji} (s⁻¹), oscillator strengths, f_{ij} , and line strengths, S_{ij} (a.u), between the ground state levels for electric quadrupole (E2) and magnetic dipole (M1) transitions in Rn III.

Transitions		λ (Å)	A_{ji} (s ⁻¹)			f_{ij}	S_{ij} (a.u)
Lower level	Upper level		This work	Other works	MCDF/Ref.[15]		
E2 Transitions							
6s ² 6p ⁴ ³ P ₂	6s ² 6p ⁴ ³ P ₁	3291.10	22.427	19.700 ^a	1.138	2.185(-8)	23.196
6s ² 6p ⁴ ³ P ₂	6s ² 6p ⁴ ³ P ₀	9088.50	0.0012	0.366 ^a	0.033	3.022(-12)	0.067
6s ² 6p ⁴ ³ P ₂	6s ² 6p ⁴ ¹ D ₂	2579.60	61.280	47.800 ^a	1.282	6.114(-8)	31.255
6s ² 6p ⁴ ³ P ₂	6s ² 6p ⁴ ¹ S ₀	1350.40	135.280	44.200 ^a	3.060	7.397(-9)	0.542
6s ² 6p ⁴ ³ P ₁	6s ² 6p ⁴ ¹ D ₂	11932.0	7.196(-3)	1.084(-3) ^a	6.638	2.560(-10)	7.772
6s ² 6p ⁴ ³ P ₀	6s ² 6p ⁴ ¹ D ₂	3602.00	2.275	2.320 ^a	0.980	2.212(-8)	6.159
6s ² 6p ⁴ ¹ D ₂	6s ² 6p ⁴ ¹ S ₀	2834.10	171.22	215.00 ^a	0.796	4.123(-8)	27.954

Table 4 Continued

M1 Transitions							
$6s^2 6p^4 \ ^3P_2$	$6s^2 6p^4 \ ^3P_1$	3291.10	480.31	530.00 ^a	0.906	4.679(-7)	1.904
$6s^2 6p^4 \ ^3P_1$	$6s^2 6p^4 \ ^3P_0$	5159.4	64.48	74.33 ^a	0.867	7.720(-7)	0.984
$6s^2 6p^4 \ ^3P_2$	$6s^2 6p^4 \ ^1D_2$	2579.60	374.65	386.00 ^a	0.970	3.737(-7)	1.192
$6s^2 6p^4 \ ^3P_1$	$6s^2 6p^4 \ ^1D_2$	11932.0	1.685	0.760 ^a	2.217	5.997(-8)	0.531
$6s^2 6p^4 \ ^3P_1$	$6s^2 6p^4 \ ^1S_0$	2290.2	2.101(3)	2.182(3) ^a	0.962	5.506(-7)	0.935

^a Ref. [15]

3.2. E2 and M1 transitions for triply ionized krypton, xenon and radon

In this study, 10039, 40520, and 41884 electric quadrupole transitions and 7238, 27585, and 30577 magnetic dipole transitions have been obtained for Kr IV, Xe IV, and Rn IV, respectively. In previous works in literature, there are the transition probabilities and a few wavelength values belong to transitions between the only ground state levels. We have compared our results for the transitions between the levels of ground state configuration of krypton, xenon and radon in Table 5, 6 and 7 for Kr IV, Xe IV and Rn IV, respectively. Except the transitions from $ns^2 np^3 \ ^2P_{1/2}$ to lower levels, we have computed the mean ratio value 1.338 for E2 transitions of Kr IV, 1.355 and 0.937 for E2 and M1 transitions of Xe IV, respectively. For Kr IV, this main ratio have been obtained the value 0.949 for M1 transitions. In Table 7, the main ratio have been found the value 1.599 and 1.248 for E2 and M1 transitions of Rn IV, respectively. There is a good agreement between obtained results and previous work results in literature, and observed values from M1 transitions are better than E2 transitions, in general. The transition probabilities from $ns^2 np^3 \ ^2P_{1/2}$ to lower levels are somewhat poor for each investigated triply ionized ion here ($n=4, 5$, and 6 , for Kr IV, Xe IV, and Rn IV, respectively). But obtained energy values of these levels have good agreement with comparison values. In our other work we submitted the energy values of Kr IV, Xe IV and Rn IV [24]. For $^2P_{1/2}$ levels, the obtained energy values are 0.29477 Ry, 0.25106 Ry and 0.42904 Ry [24] and comparison values are 0.29440 Ry [9], 0.25551 Ry [12] and 0.42599 Ry [15] for Kr IV, Xe IV and Rn IV, respectively. Therefore, we can say that the energy level values for ground state configuration of Kr IV, Xe IV and Rn IV are good agreement with other works.

The transitions with the biggest transition probability (A_{ji}) are sorted in Tables S4, S5 and S6 for Kr IV, Xe IV and Rn IV ions, respectively. The transition parameters in these tables are new.

Table 5. The wavelengths, λ (Å), transition probabilities, A_{ji} (s^{-1}), oscillator strengths, f_{ij} , and line strengths, S_{ij} (a.u), between the ground state levels for electric quadrupole (E2) and magnetic dipole (M1) transitions in Kr IV.

Transitions		λ (Å)	A_{ji} (s ⁻¹)			f_{ij}	S_{ij} (a.u)
Lower level	Upper level		This work	Other works	MCDF/Ref.[8]		
E2 Transitions							
4s ² 4p ³ 4S ^o _{3/2}	4s ² 4p ³ 2D ^o _{5/2}	4385.30	6.854(-2)	2.985(-2) ^a	2.313	2.964(-10)	0.595
				2.962(-2) ^{a*}			
4s ² 4p ³ 4S ^o _{3/2}	4s ² 4p ³ 2D ^o _{3/2}	4791.20	3.042(-2)	1.266(-2) ^a	2.423	1.046(-10)	0.274
				1.255(-2) ^{a*}			
4s ² 4p ³ 4S ^o _{3/2}	4s ² 4p ³ 2P ^o _{1/2}	3091.50	6.124	3.554(-2) ^a	1.666	4.387(-9)	3.088
				3.674(-2) ^{a*}			
4s ² 4p ³ 4S ^o _{3/2}	4s ² 4p ³ 2P ^o _{3/2}	2876.90	0.773(-3)	1.614(-3) ^a	0.408	9.590(-12)	0.005
				1.893(-3) ^{a*}			
4s ² 4p ³ 2D ^o _{5/2}	4s ² 4p ³ 2P ^o _{1/2}	10478.00	1.736(-4)	0.137 ^a	12.764	9.529(-13)	0.039
				0.136 ^{a*}			
				4.420(-2) ^b			
				1.570(-2) ^{b*}			
				8.910(-2) ^{b**}			
4s ² 4p ³ 2D ^o _{3/2}	4s ² 4p ³ 2D ^o _{5/2}	51757.00	20.686(-7)	8.233(-7) ^a	2.601	1.246(-12)	4.116
				7.953(-7) ^{a*}			
4s ² 4p ³ 2P ^o _{1/2}	4s ² 4p ³ 2P ^o _{3/2}	41455.00	2.095(-6)	2.528(-6) ^a	0.857	1.079(-12)	0.916
				2.442(-6) ^{a*}			
4s ² 4p ³ 2D ^o _{3/2}	4s ² 4p ³ 2P ^o _{1/2}	8714.20	0.039	0.351 ^a	0.112	2.232(-10)	3.519
				0.350 ^{a*}			
4s ² 4p ³ 2D ^o _{3/2}	4s ² 4p ³ 2P ^o _{3/2}	7200.60	0.101	0.257 ^a	0.397	7.816(-10)	6.952
				0.254 ^{a*}			
4s ² 4p ³ 2D ^o _{5/2}	4s ² 4p ³ 2P ^o _{3/2}	8364.30	0.183	0.496 ^a	0.369	1.277(-9)	26.718
				0.495 ^{a*}			

Table 5 Continued

M1 Transitions							
$4s^2 4p^3 \ ^4S^{\circ}_{3/2}$	$4s^2 4p^3 \ ^2D^{\circ}_{5/2}$	4385.30	0.105	0.124 ^a	0.853	4.532(-10)	0.002
				0.123 ^{a*}			
				0.151 ^b			
				0.167 ^{b*}			
				0.131 ^{b**}			
$4s^2 4p^3 \ ^4S^{\circ}_{3/2}$	$4s^2 4p^3 \ ^2D^{\circ}_{3/2}$	4791.20	3.921	3.148 ^a	1.253	1.349(-8)	0.063
				3.128 ^{a*}			
				3.340 ^b			
				3.940 ^{b*}			
				2.750 ^{b**}			
$4s^2 4p^3 \ ^4S^{\circ}_{3/2}$	$4s^2 4p^3 \ ^2P^{\circ}_{1/2}$	3091.50	11.330	12.580 ^a	0.905	8.116(-9)	0.024
				12.520 ^{a*}			
				10.100 ^b			
				9.420 ^{b*}			
				10.000 ^{b**}			
$4s^2 4p^3 \ ^4S^{\circ}_{3/2}$	$4s^2 4p^3 \ ^2P^{\circ}_{3/2}$	2876.90	21.384	23.500 ^a	0.912	2.653(-8)	0.075
				23.460 ^{a*}			
				19.300 ^b			
				17.300 ^{b*}			
				19.800 ^{b**}			
$4s^2 4p^3 \ ^2D^{\circ}_{3/2}$	$4s^2 4p^3 \ ^2D^{\circ}_{5/2}$	51757.00	6.7034(-2)	4.870(-2) ^a	1.393	4.038(-8)	2.067
				4.810(-2) ^{a*}			
				4.840(-2) ^b			
				6.820(-2) ^{b*}			
				3.580(-2) ^{b**}			

Table 5 Continued

$4s^24p^3\ ^2P^o_{1/2}$	$4s^24p^3\ ^2P^o_{3/2}$	41455.00	10.705(-2)	$9.930(-2)^a$	1.071	5.516(-8)	1.131
				$9.988(-2)^{a*}$			
				$7.600(-2)^b$			
				$10.700(-2)^{b*}$			
				$6.230(-2)^{b**}$			
$4s^24p^3\ ^2D^o_{3/2}$	$4s^24p^3\ ^2P^o_{1/2}$	8714.20	3.591	5.020^a	0.718	2.044(-8)	0.176
				4.996^{a*}			
				3.360^b			
				2.650^{b*}			
				3.830^{b**}			
$4s^24p^3\ ^2D^o_{3/2}$	$4s^24p^3\ ^2P^o_{3/2}$	7200.60	9.719	13.190^a	0.740	7.555(-8)	0.538
				13.140^{a*}			
				8.370^b			
				7.500^{b*}			
				8.930^{b**}			
$4s^24p^3\ ^2D^o_{5/2}$	$4s^24p^3\ ^2P^o_{3/2}$	8364.30	3.797	5.443^a	0.699	2.655(-8)	0.329
				5.430^{a*}			
				3.530^b			
				2.860^{b*}			
				4.030^{b**}			

^a Ref. [8]; ^b Ref. [9]

Note: *b, b*, b** values are belong to the same study, which were presented different configuration sets.*

Table 6. The wavelengths, λ (Å), transition probabilities, A_{ji} (s^{-1}), oscillator strengths, f_{ij} , and line strengths, S_{ij} (a.u), between the ground state levels for electric quadrupole (E2) and magnetic dipole (M1) transitions in Xe IV.

Transitions		λ (Å)		A_{ji} (s ⁻¹)			f_{ij}	S_{ij} (a.u)
Lower level	Upper level	This work	Other works	This work	Other works	MCDF/Ref.[12]		
E2 Transitions								
5s ² 5p ³ 4S ^o _{3/2}	5s ² 5p ³ 2D ^o _{5/2}	4936.30		0.421	0.229 ^a	1.838	2.310(-9)	6.620
5s ² 5p ³ 4S ^o _{3/2}	5s ² 5p ³ 2D ^o _{3/2}	6519.00		0.081	0.042 ^a	1.928	5.142(-10)	3.394
5s ² 5p ³ 4S ^o _{3/2}	5s ² 5p ³ 2P ^o _{1/2}	3629.7	3570.00 ^b	6.957	0.858 ^a	8.108	6.871(-9)	7.828
5s ² 5p ³ 4S ^o _{3/2}	5s ² 5p ³ 2P ^o _{3/2}	2826.30		0.021	0.017 ^a	1.235	2.481(-11)	0.013
5s ² 5p ³ 2D ^o _{5/2}	5s ² 5p ³ 2P ^o _{1/2}	13713.00		2.651(-5)	0.118 ^a	0.0002	2.492(-13)	0.023
5s ² 5p ³ 2D ^o _{3/2}	5s ² 5p ³ 2D ^o _{5/2}	20333.00		6.396(-4)	2.257(-4) ^a	2.833	5.946(-11)	11.909
5s ² 5p ³ 2P ^o _{1/2}	5s ² 5p ³ 2P ^o _{3/2}	12768.00		3.431(-3)	4.155(-3) ^a	0.825	1.676(-10)	4.158
5s ² 5p ³ 2D ^o _{3/2}	5s ² 5p ³ 2P ^o _{1/2}	8189.80		0.033	0.712 ^a	0.046	1.653(-10)	2.164
5s ² 5p ³ 2D ^o _{3/2}	5s ² 5p ³ 2P ^o _{3/2}	4989.50	4470.00 ^b	0.574	1.332 ^a	0.431	2.145(-9)	6.348
5s ² 5p ³ 2D ^o _{5/2}	5s ² 5p ³ 2P ^o _{3/2}	6612.00		0.898	2.272 ^a	0.395	3.925(-9)	40.546
M1 Transitions								
5s ² 5p ³ 4S ^o _{3/2}	5s ² 5p ³ 2D ^o _{5/2}	4936.30		2.062	2.360 ^a	0.873	1.130(-8)	0.055
5s ² 5p ³ 4S ^o _{3/2}	5s ² 5p ³ 2D ^o _{3/2}	6519.00		23.351	20.930 ^a	1.115	1.487(-7)	0.959
5s ² 5p ³ 4S ^o _{3/2}	5s ² 5p ³ 2P ^o _{1/2}	3629.7	3570.00 ^b	41.407	51.000 ^a	0.811	4.089(-8)	0.146
5s ² 5p ³ 4S ^o _{3/2}	5s ² 5p ³ 2P ^o _{3/2}	2826.30		36.967	39.330 ^a	0.939	4.427(-8)	0.123
5s ² 5p ³ 2D ^o _{3/2}	5s ² 5p ³ 2D ^o _{5/2}	20333.00		0.918	0.634 ^a	1.447	8.534(-8)	1.716
5s ² 5p ³ 2P ^o _{1/2}	5s ² 5p ³ 2P ^o _{3/2}	12768.00		2.983	2.903 ^a	1.027	1.458(-7)	0.920
5s ² 5p ³ 2D ^o _{3/2}	5s ² 5p ³ 2P ^o _{1/2}	8189.80		6.370	8.215 ^a	0.775	3.202(-8)	0.259
5s ² 5p ³ 2D ^o _{3/2}	5s ² 5p ³ 2P ^o _{3/2}	4989.50	4470.00 ^b	60.238	80.500 ^a	0.748	2.248(-7)	1.109
5s ² 5p ³ 2D ^o _{5/2}	5s ² 5p ³ 2P ^o _{3/2}	6612.00		14.522	20.670 ^a	0.703	6.345(-8)	0.622

^a Ref. [12]; ^b Ref. [11]

Table 7. The wavelengths, λ (Å), transition probabilities, A_{ji} (s^{-1}), oscillator strengths, f_{ij} , and line strengths, S_{ij} (a.u), between the ground state levels for electric quadrupole (E2) and magnetic dipole (M1) transitions in Rn IV.

Transitions		λ (Å)	A_{ji} (s ⁻¹)			f_{ij}	S_{ij} (a.u)
Lower level	Upper level		This work	Other works	MCDF/Ref.[15]		
E2 Transitions							
6s ² 6p ³ 4S ^o _{3/2}	6s ² 6p ³ 2D ^o _{5/2}	2641.80	35.609	37.000 ^a	0.962	5.588(-8)	24.551
6s ² 6p ³ 4S ^o _{3/2}	6s ² 6p ³ 2D ^o _{3/2}	3389.50	60.773	6.150 ^a	9.881	1.046(-8)	9.711
6s ² 6p ³ 4S ^o _{3/2}	6s ² 6p ³ 2P ^o _{1/2}	2124.00	140.52	86.000 ^a	1.633	4.752(-8)	10.848
6s ² 6p ³ 4S ^o _{3/2}	6s ² 6p ³ 2P ^o _{3/2}	1302.00	11.805	12.100 ^a	0.975	3.000(-8)	0.157
6s ² 6p ³ 2D ^o _{5/2}	6s ² 6p ³ 2P ^o _{1/2}	10836.00	1.727(-4)	0.132 ^a	0.001	1.013(-12)	0.046
6s ² 6p ³ 2D ^o _{3/2}	6s ² 6p ³ 2D ^o _{5/2}	11977.00	0.333(-4)	6.617(-4) ^a	0.050	1.076(-10)	4.407
6s ² 6p ³ 2P ^o _{1/2}	6s ² 6p ³ 2P ^o _{3/2}	3364.20	4.664	6.900 ^a	0.675	1.582(-8)	7.178
6s ² 6p ³ 2D ^o _{3/2}	6s ² 6p ³ 2P ^o _{1/2}	5688.80	0.043	1.305 ^a	0.033	1.046(-10)	0.459
6s ² 6p ³ 2D ^o _{3/2}	6s ² 6p ³ 2P ^o _{3/2}	2114.00	43.360	48.500 ^a	0.894	2.905(-8)	6.539
6s ² 6p ³ 2D ^o _{5/2}	6s ² 6p ³ 2P ^o _{3/2}	2567.20	119.000	138.800 ^a	0.857	7.838(-8)	47.39
M1 Transitions							
6s ² 6p ³ 4S ^o _{3/2}	6s ² 6p ³ 2D ^o _{5/2}	2641.80	100.140	113.800 ^a	0.880	1.571(-7)	0.411
6s ² 6p ³ 4S ^o _{3/2}	6s ² 6p ³ 2D ^o _{3/2}	3389.50	529.030	592.500 ^a	0.892	9.112(-7)	3.054
6s ² 6p ³ 4S ^o _{3/2}	6s ² 6p ³ 2P ^o _{1/2}	2124.00	635.580	690.000 ^a	0.921	2.149(-7)	0.452
6s ² 6p ³ 4S ^o _{3/2}	6s ² 6p ³ 2P ^o _{3/2}	1302.00	50.760	24.950 ^a	2.034	1.290(-8)	0.016
6s ² 6p ³ 2D ^o _{3/2}	6s ² 6p ³ 2D ^o _{5/2}	11977.00	3.333	1.683 ^a	1.980	1.075(-7)	1.273
6s ² 6p ³ 2P ^o _{1/2}	6s ² 6p ³ 2P ^o _{3/2}	3364.20	135.490	146.800 ^a	0.922	4.597(-7)	0.765
6s ² 6p ³ 2D ^o _{3/2}	6s ² 6p ³ 2P ^o _{1/2}	5688.80	4.566	2.580 ^a	1.769	1.107(-8)	0.062
6s ² 6p ³ 2D ^o _{3/2}	6s ² 6p ³ 2P ^o _{3/2}	2114.00	1.292(3)	1.378(3) ^a	0.937	8.658(-7)	1.810
6s ² 6p ³ 2D ^o _{5/2}	6s ² 6p ³ 2P ^o _{3/2}	2567.20	264.010	292.500 ^a	0.902	1.739(-7)	0.662

^a Ref. [15]

Conclusion

In summary, in this work, the calculations for forbidden transitions for doubly and triply ionized krypton, xenon and radon have been done using the general-purpose relativistic atomic structure package (GRASP) based on a fully relativistic multiconfiguration Dirac-Fock (MCDF) method. The calculations include Breit and QED contributions and correlation effects. In general, obtained results from these calculations and previous work results in literature are quite agreement for forbidden transitions between the ground state levels. In particular, we hope that new results obtained from this work are very important in the fields of quantum electronics, atomic and laser spectroscopy, plasma, and astrophysics, and will be useful in analyzing of the spectrum of some noble gases and support, in particular, the theoretical and experimental works in the future.

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