Theoretical Studies of Quadruply Ionized Radon (Rn V) for Energetically Low Lying Levels

B. KARAÇOBAN USTA a,* AND S. ESER^b

^a Department of Fundamental Science in Engineering, Sakarya University of Applied Science, 54050, Sakarya, Turkey
^b Department of Physics, Sakarya University, 54050, Sakarya, Turkey

Received: 22.10.2020 & Accepted: 30.01.2021

Doi: 10.12693/APhysPolA.139.132

*e-mail: bkaracoban@subu.edu.tr

We have reported the energies and transition parameters for allowed transition (electric dipole, E1), and forbidden transitions (electric quadrupole, E2, and magnetic dipole, M1) for quadruply ionized radon (Rn V, Z = 86) for energetically low lying levels. The present results were performed using two independent computational strategies of the Hartree–Fock calculation with relativistic corrections and superposition of configurations (Cowan's HFR method) and the general-purpose relativistic atomic structure package based on the fully relativistic multiconfiguration Dirac–Fock (MCDF) method. We have compared our results with the results available in the literature to assess the accuracy of the data. We predict that new energy levels and transition parameters, where no other experimental or theoretical results are available, will form the basis for future experimental work.

topics: HFR method, MCDF method, relativistic corrections, wavelengths

1. Introduction

The spectrum of noble gases is of interest for many physics areas, for example, laser physics, fusion diagnostics, photoelectron spectroscopy, collision physics, astrophysics, etc. [1]. Particularly for the ionized noble gases, the importance of reliable values of oscillator strengths is well known for the plasma diagnostics, determination of stellar abundance and atmosphere modeling, laser physics, etc. [2].

Radon is a radioactive noble gas element, which is obtained by radioactive disintegration of radium, while all other noble gases are present in atmosphere. Radon is also useful in the cancer treatment because it is radioactive in nature [3]. The quadruply ionized radon (Rn V) belongs to the Pb isoelectronic sequence. Its ground state is $6s^2 6p^{2} {}^{3}P_0$. There is less spectroscopic literature concerning Rn V than the neutral or other ionized species, namely there are only two studies. Chou et al. [4] presented oscillator strength of $6s^2 6p^{2} {}^{3}P_0 - {}^{3}P_1$ magnetic-dipole (M1) transition using the multiconfiguration relativistic randomphase approximation (MCRRPA) theory. Later, Biémont and Quinet [5] reported transition probabilities and oscillator strengths of M1 and electricquadrupole (E2) transitions among $6s^26p^2$ levels. For Rn V, there has not been any study on allowed transition parameters. Data on energies, electric-dipole (E1), E2 and M1 transitions for this ion have been presented for the first time in this work.

The aim of this paper is to obtain atomic data for quadruply ionized (Rn V Z = 86) using the relativistic Hartree–Fock (HFR) code [6] and the general-purpose relativistic atomic structure package (GRASP) code [7]. We have reported relativistic energies and the Landé g-factors for the levels of $6s^26p^2$, $6s^26p nd$ (n = 6-10), $6s^26p ns$ (n = 7-10), $6s^{2}6p nf (n = 5-10), 6s^{2}6p np (n = 7-10), 6s^{2}6p nh$ $(n = 6-10), \quad 6s^2 6p \, ng \quad (n = 6-10) \quad \text{and} \quad 6s^2 6p \, ni$ (n = 7-10) configurations and the transition parameters, such as the wavelengths, oscillator strengths and transition probabilities, for E1, E2 and M1 transitions between excitation levels in Rn V. Calculations have been carried out by the HFR method [8] and the GRASP atomic structure package based on the fully relativistic multiconfiguration Dirac–Fock (MCDF) method [9]. The HFR method considers the correlation effects and relativistic corrections. For valence excitations, we have only taken into account the configurations including one electron excitation from valence (6p orbital)to other subshells: $6s^26p^2$, $6s^26p nd$ (n = 6-10), $6s^{2}6p ns (n = 7-10), 6s^{2}6p nf (n = 5-10), 6s^{2}6p np$ $\begin{array}{ll} (n=7-10), & 6s^26p\,nh & (n=6-10), & 6s^26p\,ng \\ (n=6-10) & {\rm and} & 6s^26p\,ni & (n=7-10) & {\rm configura-} \end{array}$ $6s^26pnq$ tions outside the core $[Xe]4f^{14}5d^{10}$ in Rn \breve{V} for the HFR calculation.

The 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 in the MCDF method. In the MCDF calculation, various configurations have been considered for correlation effects. More and more electron correlations have been progressively included in the calculation. For a VV correlation, only one electron outside $6s^26p$ is considered in the calculation. In a CV correlation, effects are added by including single excitations from the 6s and 6p subshells, while a CC electron correlation contributions are considered with double excitations from 6s [10]. Thus, we have taken into account $6s^26p^2$, $6s^26p nd$ (n = 6, 7), $6s^26p ns$ (n = 7, 8), $6s^26p 5f$, $6s^26p np$ (n = 7, 8), $6p^4$, $6s^6p7d^2$, $6p^27s^2$, $6s6p5f^2$, $6s6p8s^2$, $6p^26d^2$ and $6s6p8p^2$ configurations according to the CC correlation. In this calculation, the closed shells of this ion are $1s^2 2s^2 2p^6 3s^2 3p^6 3d^{10} 4s^2 4p^6 4d^{10} 4f^{14} 5s^2 5p^6 5d^{10}$.

2. Calculation methods

The relativistic Hartree–Fock method developed by Cowan (Cowan's HFR method) [8] and the fully relativistic MCDF method developed by Grant [9] are applied, which has been successfully done in our previous works [11–20], to perform these large-scale calculations. Since a detailed explanation of these methods has been presented in [8, 9], consequently only a brief outline is discussed here.

In the HFR method [8], for N-electron atom of nuclear charge Z_0 , the Hamiltonian is expanded as

$$H = -\sum_{i} \nabla_{i}^{2} - \sum_{i} \frac{2Z_{0}}{r_{i}} + \sum_{i>j} \frac{2}{r_{ij}} + \sum_{i} \zeta_{i}(r_{ij})\boldsymbol{l}_{i} \cdot \boldsymbol{s}_{i}$$
(1)

with r_i — the distance of the *i*-th electron from the nucleus and $r_{ij} = |\mathbf{r}_i - \mathbf{r}_j|$. Distances are measured in the Bohr units $[a_0]$ and all energies are measured in the Rydberg units [Ry]. The spin–orbit term (in Ry) is $\zeta_i(R) = \frac{\alpha^2}{2} \frac{1}{r} \left(\frac{\partial V}{\partial r}\right)$, with α being the fine structure constant and V — the mean potential field due to the nucleus and other electrons. The wave function $|\gamma JM\rangle$ of the M sublevel of a level labeled γJ is expressed in terms of LS basis states $|\alpha LSJM\rangle$ by

$$|\gamma JM\rangle = \sum_{\alpha LS} |\alpha LSJM\rangle \langle \alpha LSJ|\gamma J\rangle \tag{2}$$

In the MCDF method [9], an atomic state can be expanded as a linear combination of configuration state functions (CSFs):

$$\Psi_a(PJM) = \sum_{r=1}^{n_c} C_r(\alpha) |\gamma_r(PJM)\rangle, \qquad (3)$$

where n_c is the number of CSFs included in the evaluation of atomic state functions and C_r is the mixing coefficient. The CSFs are the sum of products of single-electron Dirac spinors

$$\phi(r,\theta,\varphi,\sigma) = \frac{1}{r} \left(\begin{array}{c} P(r)\chi_{\kappa m}(\theta,\varphi,\sigma) \\ iQ(r)\chi_{-\kappa m}(\theta,\varphi,\sigma) \end{array} \right), \quad (4)$$

where $j = |\kappa| - 1/2$ is the relativistic angular quantum number (note that $\kappa = \pm (j + 1/2)$ for $l = (j \pm 1/2)$) and $\chi_{\kappa m}$ is the spinor spherical harmonic in the *LSJ* coupling scheme and *P*(*r*) and *Q*(*r*) are the large and small radial components of one-electron wave functions represented on a logarithmic grid.

The energy functional is based on the Dirac–Coulomb Hamiltonian for an N-electron atom in the form

$$H_{DC} = \sum_{j=1}^{N} \left(c \boldsymbol{\alpha}_{j} \cdot \boldsymbol{p}_{j} + (\beta_{j} - 1)c^{2} + V(r_{j}) \right)$$
$$+ \sum_{i < k}^{N} \frac{1}{r_{jk}}, \tag{5}$$

where $V(r_j)$ is the electron-nucleon interaction and c is the speed of light.

3. Results and discussion

In this paper, we have calculated the relativistic energies and the Landé g-factors for the levels of $6s^26p^2$, $6s^26p nd$ (n = 6-10), $6s^26p ns$ (n = 7-10), $6s^{2}6pnf$ (n = 5–10), $6s^{2}6pnp$ (n = 7–10), $6s^{2}6pnh$ $(n = 6-10), 6s^2 6p nq (n = 6-10) \text{ and } 6s^2 6p ni$ (n = 7-10) configurations and the transition parameters (wavelengths, oscillator strengths and transition probabilities) for E1, E2 and M1 transitions between low-lying levels in Rn V using the HFR [6] and GRASP [7] codes. The configuration sets selected for investigating correlation effects have been given in Sect. 1. The results in this work are given in Tables I–II and compared with the available data. Odd-parity states only are indicated by the superscript 'o'. References for other comparison values are typed with a superscript lowercase letter. Also, the new results of this work are given in the supplementary material [21] in Tables SI, SII and SIII.

We have presented our calculations using the RCN, RCN2, RCG and RCE chain of programs developed by Cowan [8]. The HFR option of the RCN code was used to derive initial values of the parameters with appropriate scaling factors in the RCN2 code. The RCE can be used to vary the various radial energy parameters E_{av} , F^k , G^k , ζ , and R^k to make a least-squares fit of experimental energy levels by an iterative procedure. The resulting least-squares fit parameters can then be used to repeat the RCG calculation with the improved energy levels and wave functions [8].

In the HFR calculation, the Hamiltonian calculated eigenvalues were not optimized to the observed energy levels via a least-squares fitting

Energies E and Landé $g\mbox{-}{\rm factors}$ for low-lying levels in Rn V.

TABLE I

Levels			g-factor		
Conf		LIED	MODE	Other	LIED
Conf.	Ierm	HFK	MCDF	works	HFK
$6s^26p^2$	${}^{3}P_{0}$	0.00	0.00	0.00	0.00
$6s^26p^2$	${}^{3}P_{1}$	34797.18	33018.87	33979^{a}	1.501
				33796^{b}	
$6s^26p^2$	${}^{1}D_{2}$	39964.11	39760.17	39449^{a}	1.215
$6s^26p^2$	${}^{3}P_{2}$	79131.41	77353.40	77700 ^a	1.286
$6s^26p^2$	${}^{1}S_{0}$	92928.29	91966.63	91852^{a}	0.00
$6s^26p(^2P)6d$	${}^{3}F_{2}^{o}$	167825.09	165683.16	-	0.754
$6s^26p(^2P)6d$	${}^{3}F_{3}^{o}$	178877.88	177519.38	_	1.118
$6s^26p(^2P)6d$	${}^{3}D_{2}^{o}$	178976.89	178396.12	_	1.259
$6s^26p(^2P)6d$	$^{3}D_{1}^{o}$	180016.22	180373.46	_	0.824
$6s^26p(^2P)6d$	${}^{3}F_{4}^{o}$	213642.51	210441.33	-	1.251
$6s^26p(^2P)6d$	${}^{1}D_{2}^{o}$	213732.79	211266.62	_	0.998
$6s^26p(^2P)6d$	${}^{3}D_{3}^{o}$	217777.99	216847.25	-	1.222
$6s^26p(^2P)6d$	${}^{3}P_{0}^{o}$	219373.89	218859.10	-	0.00
$6s^26p(^2P)6d$	${}^{3}P_{1}^{o}$	219564.28	219383.50	-	1.197
$6s^26p(^2P)6d$	${}^{3}P_{2}^{o}$	221127.21	221002.27	-	1.323
$6s^26p(^2P)6d$	$^{1}P_{1}^{o}$	227834.29	241377.31	-	1.106
$6s^26p(^2P)6d$	${}^{1}F_{3}^{o}$	231175.19	234934.46	-	1.078
$6s^26p(^2P)7s$	${}^{3}P_{0}^{o}$	186968.69	183842.06	_	0.00
$6s^26p(^2P)7s$	$^{3}P_{1}^{o}$	188205.80	184794.35	-	1.327
$6s^26p(^2P)7s$	$^{3}P_{2}^{o}$	230374.10	226887.30	_	1.501
$6s^26p(^2P)7s$	$^{1}P_{1}^{o}$	238188.89	225469.92	_	1.047
$6s^{2}6p(^{2}P)5f$	${}^{3}G_{3}$	194823.89	198489.63	_	0.831
$6s^26p(^2P)5f$	$^{3}F_{3}$	199932.08	239307.18	_	1.172
$6s^26p(^2P)5f$	$^{3}G_{4}$	201206.70	249150.52	_	1.100
$6s^26p(^2P)5f$	${}^{3}F_{2}$	201408.50	208371.03	_	0.838
$6s^{2}6p(^{2}P)5f$		235314.29	-	-	0.959
$6s^{2}6p(^{2}P)5f$	F_4	237575.70	329733.07	_	1.169
$6s^{2}6p(^{2}P)5f$		238184.08	331529.04	_	1.200
$6s^{2}6p(^{2}P)5f$	$^{\circ}D_{3}$	240729.51	287545.52	_	1.205
$6s^{-}6p(^{-}P)5f$	$^{\circ}D_2$	241050.49	247131.95	_	0.991
$6s^{-}6p(^{-}P)5f$	$^{\circ}D_{1}$	243180.70	249087.16	_	0.499
$0s \ 0p(P) 0f$		248880.77	222067.05	_	1.031
$6s^{2}6n(^{2}P)7n$	D_2	201160.01	217082.45	_	1.009
$6s^{2}6n(^{2}P)7n$	D_1	221008.81	217062.45	_	0.007
$6s^{2}6n(^{2}P)7n$	r_0	227110.57	220091.40	_	0.000
$6s^{2}6n(^{2}P)7n$	$3D_{2}$	235390.00	230810.10	_	1.400
$6s^{2}6n(^{2}P)7n$	D_2	267811 21	262041 48		1.171
$6s^{2}6n(^{2}P)7n$	$1 D_{2}$	268521.20	264105 10		1.304
$6s^{2}6n(^{2}P)7n$	$^{3}D_{2}$	200521.29	272553.01	_	1.200
$6s^26n(^2P)7n$	$1 P_1$	278/27.01	272555.01	_	1.505
$6s^26n(^2P)7n$	1	281133 31	276733.14	_	1.000
$6s^26n(^2P)7n$	$1 \frac{1}{S_{c}}$	286072.20	210135.14	_	0.000
$6s^26n(^2P)$	$3 P_{\circ}^{o}$	287829 08	281890 56	_	0.000
$6s^{2}6n(^{2}P)8s$	$^{3}P^{o}$	288334 50	282250 17	_	1 394
$6s^26n(^2P)8s$	$^{-1}_{3}P_{2}^{o}$	332286 10	326266.89	_	1.488
$6s^2 6p(^2P)8s$	$^{1}P_{1}^{o}$	333704.09	326578.22	_	1.047
	- 1	1	1	I	

Levels		$E [\mathrm{cm}^{-1}]$			g-factor
Conf.	Term	HFR	MCDF	Other works	HFR
$6s^26p(^2P)8p$	$^{3}D_{1}$	303982.02	298373.22	—	0.665
$6s^26p(^2P)8p$	${}^{3}P_{0}$	306193.09	302714.12	—	0.00
$6s^26p(^2P)8p$	${}^{3}S_{1}$	310163.50	304976.05	_	1.487
$6s^26p(^2P)8p$	$^{3}D_{2}$	310385.07	305530.60	_	1.171
$6s^26p(^2P)8p$	${}^{3}P_{1}$	349070.07	343386.13	_	1.380
$6s^26p(^2P)8p$	$^{1}D_{2}$	349638.59	344193.37	_	1.212
$6s^26p(^2P)8p$	$^{3}D_{3}$	354141.07	348167.79	_	1.333
$6s^26p(^2P)8p$	$^{1}P_{1}$	354360.32	348651.46	_	1.474
$6s^26p(^2P)8p$	$^{3}P_{2}$	355167.82	350446.39	_	1.283
$6s^26p(^2P)8p$	${}^{1}S_{0}$	357812.99	355503.00	_	0.00
$6s^26p(^2P)7d$	${}^{3}F_{2}^{o}$	283557.18	278004.88	_	0.768
$6s^26p(^2P)7d$	${}^{3}D_{1}^{o}$	286076.21	-	—	0.828
$6s^26p(^2P)7d$	${}^{3}P_{2}^{o}$	286445.53	281888.70	—	1.277
$6s^26p(^2P)7d$	${}^{3}F_{3}^{o}$	287109.37	283410.08	_	1.118
$6s^26p(^2P)7d$	$^{1}D_{2}^{o}$	327857.90	321879.32	—	0.981
$6s^26p(^2P)7d$	$^{3}D_{3}^{o}$	328897.67	323625.73	—	1.188
$6s^26p(^2P)7d$	${}^{3}F_{4}^{o}$	329506.93	323810.18	_	1.250
$6s^26p(^2P)7d$	${}^{3}P_{1}^{o}$	329557.72	324749.22	—	1.087
$6s^26p(^2P)7d$	${}^{3}D_{2}^{o}$	330185.54	_	—	1.320
$6s^26p(^2P)7d$	${}^{3}P_{0}^{o}$	330186.49	325743.63	_	0.000
$6s^26p(^2P)7d$	${}^{1}F_{3}^{o}$	331914.61	329761.37	_	1.117
$6s^26p(^2P)7d$	$^{1}P_{1}^{o}$	332126.49	332666.64	_	1.194

^{*a*}Ref. [5], ^{*b*}Ref. [4]

procedure using experimentally determined energy levels (in RCE) since the experimentally determined energy levels are not available in the literature for Rn V. The scaling factors of the Slater parameters $(F^k \text{ and } G^k)$ and of configuration interaction integrals (R^k) , not optimized in the least-squares fitting, were chosen as equal to 0.75 for calculation, while the spin-orbit parameters were left at their initial values. This value of the scaling factors was suggested by the Cowan range from about 0.7 or 0.8 for neutral or weakly ionized systems [6, 8]. It is known empirically that scaling down of the HF Coulomb radial integral values by 5 to 20 percent will give RCG eigenvalues in better agreement with experimental energy levels, the smaller factors being for neutral or weakly ionized systems [8]. The calculated HFR results are reported in the tables as abinitio results.

The relativistic energies and the Landé g-factors of $6s^26p^2$, $6s^26pnd$ (n = 6, 7), $6s^26pns$ (n = 7, 8), $6s^26p5f$ and $6s^26pnp$ (n = 7, 8) configurations in Rn V are presented in Table I for the HFR and MCDF results. The obtained results have given energies $[cm^{-1}]$ relative to $6s^26p^2$ ${}^{3}P_0$ ground-state level. The energies of $6s^26p^2$ configuration have been compared with other results [4, 5] in Table I. Comparison values are only available in the literature for five levels. Chou et al. [4] presented only energy of $6s^26p^2$ 3P_1 using the multiconfiguration relativistic random-phase-approximation theory (MCRRPA). Biémont and Quinet [5] calculated the energy levels and radiative transition probabilities for states within the $6p^k$ (k = 1-5) configurations in the thallium, lead, bismuth, polonium and actinium sequences up to radon using the relativistic Hartree–Fock method. In [5], according to the level compositions (LS coupling), ${}^{3}P_{2}$ and ${}^{1}D_{2}$ have been interchanged for Rn V. Although the dominant component of the eigenvector corresponds to ${}^{1}D_{2}$, it has been determined as ${}^{3}P_{2}$ in [5]. A similar situation is for the other level. According to our studies with both methods, ${}^{3}P_{2}$ and ${}^{1}D_{2}$ should be interchanged. When such a comparison is made, our results for the energies of these two levels appear to be in good agreement with [5].

To interpret the accuracy of our results, we used ($|E_{\rm this\ work}-E_{\rm other\ works}|/E_{\rm other\ works}$) × 100%. The comparison between our results and theoretical [4, 5] has showed the differences in energies in the range of 0.12–2.83% when using the HFR and MCDF calculations. As seen in Table I, the results obtained from the HFR and MCDF calculations are in agreement with each other for $6s^{2}6p nd (n = 6, 7), 6s^{2}6p ns (n = 7, 8), 6s^{2}6p 5f$ and $6s^{2}6p np (n = 7, 8)$ configurations. These data for Rn V have been for the first



Fig. 1. Comparison of the wavelengths obtained from this work (the HFR and MCDF calculations) for E1 transitions.



Fig. 2. Comparison of the logarithmic weighted oscillator strengths obtained from this work (the HFR and MCDF calculations) for E1 transitions.

time presented in this work. Also, for high-lying levels $(6s^26p nd (n = 8-10), 6s^26p ns (n = 8-10), 6s^26p nf (n = 6-10), 6s^26p np (n = 9, 10), 6s^26p nh (n = 6-10), 6s^26p ng (n = 6-10) and 6s^26p ni (n = 7-10))$, energies and the Landé g-factors obtained using the HFR code are given in Table SI provided in the supplementary material [21].

Here, the data on E1 transitions for this ion have been for the first time presented using the HFR and MCDF methods. We have obtained 13,956 and 22,636 possible E1 transitions, respectively. The wavelengths λ [Å], logarithmic weighted oscillator strengths, $\log(gf)$, and transition probabilities, A_{ji} [s⁻¹], for $6s^26p^2-6s^26p6d$, $6s^26p^2-6s^26p7s$, $6s^26p6d-6s^26p7p$ and $6s^26p7s-6s^26p7p$ E1 transitions between low-lying levels obtained using the HFR [6] and GRASP [7] codes are presented in Table SII provided in [21]. Figures 1–3 also show the HFR and MCDF methods comparison for E1 transitions. Linear correlation coefficient R^2 is 0.98 for wavelengths and 0.96 for logarithmic weighted oscillator strengths and transition probabilities. The agreement between the presented data is a strong evidence for the reliability of the HFR and MCDF calculations. Figure 3 does not include the transition probability values of smaller than or equal to 10^6 and greater than or equal to 10^{10} .



Fig. 3. Comparison of the transition probabilities obtained from this work (the HFR and MCDF calculations) for E1 transitions.

To date, there have been only two studies on the forbidden transition parameters for Rn V. These are M1 and E2 transitions among $6s^26p^2$ levels [4, 5]. Chou et al. [4] reported oscillator strength of $6s^26p^{23}P_0^{-3}P_1$ M1 transition using the MCR-RPA. Biémont and Quinet [5] presented calculation results for nine transitions of Rn V using the HFR. We obtained 21,082 for E2 and 13,830 for M1 transitions in the HFR calculation and 38,369 for E2 and 26,973 for M1 transitions in the MCDF calculation. Table II reports wavelengths λ [Å], transition probabilities A_{ji} [s⁻¹], and logarithmic weights oscillator strengths $\log(qf)$, between the ground state levels $(6s^26p^2)$ for forbidden (E2 and M1) transitions in Rn V. We have compared our results with those reported by Biémont and Quinet [5] for nine transitions in Table II. A good agreement of our results with both these results has been observed. As seen in Table II, the results obtained from the HFR and MCDF calculations are in agreement with each other for wavelengths and logarithmic weighted oscillator strengths results. Some small difference has arisen from the fact that the methods involved different contributions.

We have calculated the mean ratio for the accuracy of our results. The values 1.04 and 0.99 (for M1 transition) and 1.04 and 0.98 (for E2 transition) are found for the mean ratio of $\lambda_{(\text{HFR})}/\lambda_{(\text{MCDF})}$ and $\log(gf)_{(\text{HFR})}/\log(gf)_{(\text{MCDF})}$, respectively. The results for transition probabilities are in agreement with [5]. For M1 transitions, the mean ratio between our results and [5] has been found in values 1.01 for the HFR calculation and 1.15 for the MCDF calculation. We have found values 1.07 (calculation HFR) and 0.89 (calculation MCDF) for the mean ratio of A_{ji} (this work)/ A_{ji} [5] for E2 transitions, except for the transition 14834.00 Å (for MCDF).

In the case for new $6s^26p^2-6s^26p7p$, $6s^26p7p-6s^26p7p$, $6s^26p6d-6s^26p6d-6s^26p6d$ and $6s^26p7s-6s^26p7s$ E2 and M1 transitions obtained from the HFR and MCDF calculations, we have also given wavelengths λ , logarithmic weighted oscillator strengths $\log(gf)$, and

Transitions		Method	λ [Å]	$A_{ji} [\mathrm{s}^{-1}]$		$\log(gf)$	
				This work	Other w.	This work	Other w.
${}^{3}P_{0} - {}^{3}P_{1}$	M1	HFR	2873.80	5.88(2)	$5.50(2)^{a}$	-5.660	-5.677^{b}
		MCDF	3028.60	4.90(2)		-5.694	
${}^{3}P_{1} - {}^{1}S_{0}$	M1	HFR	1720.25	2.410(3)	$2.330(3)^a$	-5.971	—
		MCDF	1696.40	2.295(3)		-6.004	
${}^{3}P_{0} - {}^{1}D_{2}$	E2	HFR	2502.24	3.43(1)	$3.140(1)^a$	-6.793	—
		MCDF	2515.10	2.86(1)		-6.868	
${}^{3}P_{0} - {}^{3}P_{2}$	E2	HFR	1263.72	5.68(0)	$4.12(0)^{a}$	-8.167	—
		MCDF	1292.80	5.33(0)		-8.175	
${}^{1}D_{2} - {}^{1}S_{0}$	E2	HFR	1888.07	4.15(2)	$3.84(2)^{a}$	-6.654	_
		MCDF	1915.50	5.05(2)		-6.556	
${}^{3}P_{2} - {}^{1}S_{0}$	E2	HFR	7248.00	1.125(0)	$1.280(0)^{a}$	-8.052	_
		MCDF	6843.10	0.049		-9.483	
${}^{3}P_{1} - {}^{1}D_{2}$	M1	HFR	19353.73	8.03(-1)	$9.72(-1)^a$	-6.647	—
		MCDF	14834.00	1.94(0)		-6.494	
	E2	HFR	19353.73	0.77(-3)	$1.030(-3)^a$	-9.664	—
		MCDF	14834.00	3.49(-3)		-9.238	
${}^{3}P_{1} - {}^{3}P_{2}$	M1	HFR	2255.59	6.73(2)	$6.34(2)^{a}$	-5.591	—
		MCDF	2255.60	5.94(2)		-5.644	
	E2	HFR	2255.59	4.65(1)	$4.14(1)^{a}$	-6.752	—
		MCDF	2255.60	3.71(1)		-6.848	
${}^{3}P_{2} - {}^{1}D_{2}$	M1	HFR	2553.15	5.980(2)	$5.60(2)^{a}$	-5.534	_
		MCDF	2660.10	5.168(2)		-5.562	
	E2	HFR	2553.15	7.304(1)	$6.320(1)^a$	-6.447	_
		MCDF	2660.40	5.704(1)		-6.519	

The wavelengths λ , transition probabilities A_{ji} and logarithmic weights oscillator strengths $\log(gf)$ between the ground state levels $(6s^26p^2)$ for forbidden (E2 and M1) transitions in Rn V.

^aRef. [5], ^bRef. [4]

transition probabilities A_{ji} and presented them in Table SIII [21]. We have found values 1.00, 1.00 and 0.98 (of E2 transitions), and 1.03, 0.99 and 1.05 (of M1 transitions) for the mean ratio of $\lambda_{(\text{HFR})}/\lambda_{(\text{MCDF})}$, $\log(gf)_{(\text{HFR})}/\log(gf)_{(\text{MCDF})}$ and $A_{ji(\text{HFR})}/A_{ji(\text{MCDF})}$, respectively. Again, the agreement between data used in this work is a strong evidence for the reliability of the HFR and MCDF calculations.

4. Conclusion

The main purpose of the present manuscript has been to obtain appropriate values determining the spectrum of Rn V. The energies and Landé g-factors for excited levels, and E1, E2 and M1 transitions are reported in Tables I–II and Tables SI–SII. Also, we have presented new results obtained from this work as supplementary tables (Tables SI-SIII). The E1, E2, and M1 transitions of Rn V have been obtained for the first time for transitions between low-lying levels, except for transitions in Table II. We hope that our results obtained using the HFR and MCDF methods will be useful for experimental studies and for interpreting the spectrum of Rn V.

Acknowledgments

The authors are very grateful to the anonymous reviewers for stimulating comments and valuable suggestions which resulted in improving the presentation of this paper.

References

- R.J. Peláez, M. Ćirišan, S. Djurović, J.A. Aparicio, S. Mar, Astron. Astrophys. 507, 1697 (2009).
- [2] F. Bredice, M. Raineri, J. Reyna Almandos, M. Gallardo, A.G. Trigueiros, J. Quant. Spectrosc. Radiat. Transf. 65, 805 (2000).
- [3] Z. Zdrojewicz, J. Strzelczyk, Int. Dose Response Soc. 4, 106 (2006).
- [4] H.-S. Chou, K.-N. Huang, W.R. Johnson, *Phys. Rev. A* 44, R2769 (1991).
- [5] E. Biémont, P. Quinet, *Phys. Scr.* 54, 36 (1996).
- [6] C. McGuinness, *R.D. Cowan's Atomic* Structure Code, 2009.

- [7] K.G. Dyall, I.P. Grant, C.T. Johnson, F.A. Parpia, E.P. Plummer, *Comp. Phys. Commun.* 55, 425(1989).
- [8] R.D. Cowan, The Theory of Atomic Structure and Spectra, Univ. of California Press, Berkeley (CA) 1981.
- [9] I.P. Grant, Relativistic Quantum Theory of Atoms and Molecules, 1st ed., Springer, New York 2007.
- [10] P. Quinet, J. Quant. Spectrosc. Radiat. Transf. 145, 153 (2014).
- [11] B. Karaçoban Usta, S. Eser, Acta Phys. Pol. A 137, 1187 (2020).
- [12] B. Karaçoban Usta, S. Eser, Acta Phys. Pol. A 137, S1 (2020).
- [13] B. Karaçoban Usta, Can. J. Phys. 97, 828 (2019).
- [14] B. Karaçoban Usta, E. Şirin Yıldırım, AIP Conf. Proc. 2042, 020017 (2018).

- [15] B. Karaçoban Usta, E. Şirin Yıldırım, AIP Conf. Proc. 2042, 020018 (2018).
- [16] B. Karaçoban Usta, B. Alparslan, Can. J. Phys. 95, 1103 (2017).
- [17] S. Eser, L. Özdemir, Ind. J. Phys. 94, 1875 (2020).
- [18] S. Eser, L. Özdemir, Can. J. Phys. 97, 529 (2019).
- [19] S. Eser, L. Özdemir, Can. J. Phys. 96, 664 (2018).
- [20] S. Eser, L. Özdemir, Acta Phys. Pol. A 133, 1324 (2018).
- [21] B. Karaçoban Usta, S. Eser, Acta Phys. Pol. A 139, 132.S1 (2021), the supplementary material with the calculated results presented in Tables SI–SIII, available online only.