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Theoretical Investigation of Rydberg Energy, Quantum Defect, Radius and Radiative Lifetime of Be III

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Abstract- The Rydberg Series and Radiative transitions in Beryllium ions have been investigated using the single-electron approximation i.e. Weakest bound electron potential model theory (WBEPMT) and quantum defect theory. The Martin expression was applied to evaluate energies and quantum defects of Rydberg levels of Be III up to n = 50. The lifetime of 157 levels have been calculated using transition probabilities of the radiative transitions. The necessary data was taken from NIST database. The radii of Rydberg levels have also been calculated.

Keywords- Rydberg Atom, Martin Formula, Be III, Rydberg Energy, Quantum Defect

I. INTRODUCTION

Beryllium (Be) is a chemical element with atomic number four, is a highly toxic divalent element on the periodic table, it is found to be a significant element for industrial use due to its uncommon metallic characteristics in comparison with aluminum and steel [1]. Beryllium is widely employed in the manufacturing materials of aeronautical industry and electronics appliances. Due to its very small neutron cross-section, it is widely employed in the manufacturing of nuclear weapons [2-4]. The Rydberg atom is a gentle giant. They occur when electrons with very high energies become excited states with very high principal quantum numbers (n). The existence of the Rydberg series was first discovered in 1885 on the basis of wavelengths of light associated with the transitions of hydrogen atoms are estimated by a simple formula proposed by Johann Balmer. Rydberg atom have large principal quantum number that there electric dipole moments interact with each other that why it have many special properties and moreover are very sensitive to electric and magnetic field that produce exaggerated responses, such as the classical trajectories of electrons around the nucleus and relatively long decay times [5]. In 1969 Anderson et al carefully measured the Lifetimes of excited states of both species of beryllium by using the foil-excitation technique. Heavy ion accelerator or electromagnetic isotope separator were used to produce ion beams from 60 to 400 keV and investigated wavelength region between 1600-7000 Å. They also studied low-lying states in Be with same technique and found average lives of eleven states in Be-I, nine in Be-II, and one in Be-III [6]. Production of double ionized beryllium ions with the beam foil technique and HFS coupling constant to determine ls2p 3P level in Be III by the zero-field quantum beat technique was proposed by Poulsen and Subtil (1974) [7]. In 1975 Bruch and Andra investigated group of metastable auto ionizing levels in beryllium, when Be^+ ion bombarded at 300 keV incident ion energy. Two peaks appearing at 102.7 and 106.7 eV, which is related to Auger decay of the Be-I ($1s2s2p^2$) $^5P^e$ term. Lifetimes of the $(1s2p^2)^4P^e$ state in Be II and the $(1s2s2p^2)^5P^e$ state in Be-I have also been determined [8]. Recently Andersen et al. reported the measurements in double ionized beryllium ions for super-narrow two-electron (2, 3*c*) $^3P^o$ and (2, 4*c*) $^3P^o$ states and also use beam foil excitation technique to measured the optical decays (2, 2*a*) ^3P-(2, 3*c*) $^3P^0$ and (2, 2*a*) ^3P-(2, 4*c*)$^3P^0$ in the extreme UV region. In 1982 Bruch presented a study about decay channels of the (2, 3*c*) $^3P^0$ and (2, 4*c*) $^3P^0$ levels in Be III and their fundamental properties [9]. Chou and Cohen worked on the structural and electronic properties of beryllium with An *ab initio* calculation, which is self-consistent pseudo potential approach of local-density-functional scheme and found good agreement between experimental and predicted values of lattice constants, electronic band structure, cohesive energy, Poisson's ratio, bulk modulus, density of states, and charge density[10].

Dhia Elhak Salhi provide calculations of energy levels, radiative rates and oscillator strengths of all types of transitions for He-like Ne and also calculate radiative lifetimes by using GRASP CODE [11]. Zhan-Bin Chen et al, estimate level energies, line strengths, wavelengths, lifetimes, oscillator strengths, radiative transition rates and hyperfine structures are numerically identified by the application of multi-configuration Dirac–Hartree–Fock (MCDHF) method and the second-order many-body perturbation theory (MBPT) method [12]. K. Wang et al, reported calculations for Be-like ions for energy levels, wavelengths, oscillator strengths, line strengths, and radiative rates for transitions among the lowest 116 fine-structure levels by using combined configuration interaction and MBPT method [13]. Zhan-Bin Chen et al optimized energy levels, oscillator strengths, wavelengths, transition probabilities and radiative rates for Ge-like ions ($49 \leq Z \leq 58$) among the lowest 88 fine-structure are calculated using the fully relativistic MCDHF and the MBPT method [14]. K. Wang calculated energy levels, radiative rates, wavelengths, line strengths and oscillator strengths among the 359 levels in the nitrogen-like atoms by using combined relativistic configuration interaction and MBPT method [15]. C.Y. Zhang calculated excitation energies, lifetimes, wavelengths and transition rates for the lowest 389 levels of F-like Kr XXVIII by using second-order MBPT and MCDHF [16]. Fatma El-Sayed et al employed general-purpose relativistic atomic structure package (GRASP) to calculate the lifetimes, fine-structure energy levels and transition probabilities for the lowest 218 levels of in Sc-XIII. [17]. Rizwana developed GUI on spreadsheet to evaluate energies, quantum defects and radii of Rydberg atom/ion and found difference of 1 cm^{-1} by tested it on various atom/ion [18]. Rizwana evaluated transition probabilities of Li I from np to ms transition ($n = 1–15$ and $m = 2, 3, 4, \& 5$) and found good agreement with previously published data [19]. M. Saeed computed lifetime, oscillator strength and line strength of ns, np, nd and nf Rydberg states by of Be II (1s2 nl), where n is up to 30 [20]. M Saeed determine the oscillator strength, line strength and transition probabilities of C IV and found difference about 7% with NIST data. Sixth-degree polynomial function of lifetime of the first 25 levels of the Rydberg Series ns, np,nd, nf, and ng was also calculated [21]. Rizwana evaluated lifetime of 196 multiplets of series 1s2 ns, 1s2 np, 1s2 nd, and 1s2 nf of N V and then compare with Biemont data [22]. For calculation of lifetime three-degree polynomial were also presented [23]. M saeed calculated transition probabilities, lifetime and quantum defect using extended Ritz formula for ns, np, nd, and nf level of Lithium [24].

II. COMPUTATIONAL ANALYSES

In weakest bound electron potential model theory (WBEPMT) the electron are revolving around the core of remaining electron and nucleus of an atom which is which is referred as Hydrogen atom. The two types of electrons in WBEPMT are weakest bound electron (WBEs) and non-weakest bound electron (NWBEs) [25]. The WBE is the electron that is most likely to ionize or to be stimulated, while the remaining electrons are known as NWBEs. Martin expression give the good approximation for single valence electron system or WBE. For NWBE's system the result are not appreciable good. We apply same assumption for Beryllium-4 for calculating quantum defect of all levels. The properties of an electron in the field of a positive ion, and specifically how to define such qualities in terms of analytical functions of the energy, are the focus of quantum defect theory (QDT). It offers a comprehensive theory of bound states that takes into account specific area, series perturbations, and elastic and inelastic electron-ion scattering [26-27]. The formula for quantum defect δ_n and is given as:

$$\delta_n = \mathrm{a} + \frac{\mathrm{b}}{(\mathrm{n} - \delta\mathrm{o})^2} + \frac{\mathrm{c}}{(\mathrm{n} - \delta\mathrm{o})^4} + \cdots \quad (1)$$

Here, δ_0 is the lowest value of quantum defect. The variables a, b, c, and d can be calculated by fitting the first few energies of Rydberg levels. The energy E of the WBE is given as:

$$E^* = -\frac{1}{2}\left(\frac{Z^+}{n^+}\right)^2 \quad (2)$$

Here in equation (2), $n^+$is the effective principle quantum number. The transformation between the Eigen value of quantum defect theory (QDT) and WBEPMT is used to determine the values of z^+ and n^+ then put these values to equation (2) to get:

$$E^* = -\frac{1}{2}\left(\frac{z_{net}}{(\mathrm{n} - \delta\mathrm{o})}\right)^2 \quad (3)$$

Here, Z_{net} is the ion-core charge number in (QDT). The ionization limit (I_{limit}) and the energy of the WBE (E^*) are added together to get the energy (E) of the unperturbed level

$$\mathrm{E} = I_{limit} + E^* \quad (4)$$

Put equation (3) in this to get,

$$\mathrm{E} = I_{limit} - \frac{1}{2}\left(\frac{z_{net}}{(\mathrm{n} - \delta\mathrm{o})}\right)^2 \quad (5)$$

From this equation we get the unperturbed Rydberg energy of (Be III) and for the expectation of radius ⟨r⟩ we use,

$$\langle \mathrm{r} \rangle = \frac{3n^+ - l^+(l^+ + 1)}{Rz^+} \quad (6)$$

Here, l^+ is the effective orbital quantum number and R is the rydberg constant which is taken $109737 cm^{-1}$ The transition probability A_{fi} of a transition for spontaneous emission between states (n_f , l_f) and (n_i , l_i) is taken from Nation institute of standards and

technology (NIST) and use it to calculate the radiative lifetime which is the reciprocal of transition probability A_{fi} of a transition for spontaneous emission between states (n_f , l_f) and (n_i , l_i), is given as.

$$\tau_f = (\sum_i A_{fi})^{-1} \quad (7)$$

III. Results and Discussion

In the past, spectral research on singly ionized elements from various families was conducted in the field. The theoretical approach known as WBEPM theory, which provides a very close relationship with the previously published unique data listed at National institute of standards and technology (NIST), is used to explore the spectrum properties of quantum defects, Radius, Rydberg energy of unperturbed series and Radiative Lifetimes of Be III shown in tables 1 to 16. Calculations are made for the Quantum defect and Rydberg energy level series with configurations $1s^2nl$ where, l = s, p, d, and f. The configuration of series is 1sns $1S_0$, 1sns $3S_1$, 1snp $1P_1^0$, 1snp $3P_{0,1,2}^0$ J (spin-orbital coupling), 1snd $1D_2$, 1snd $3D_{1,2,3}$, 1snf $1F_3^0$ and 1snf $3F_{2,3,4}^0$ Shown in table 12,13,14,15 and 16 (In Appendix). For calculation we took four energy levels of Be III listed at NIST entered into a python-based software. The data for the quantum number (n) up to n=50 is generated by this software based on above mentioned equations in the theory. From the extracted data we draw the graphs of Rydberg energy of Be III, quantum defect and radius. In the graphs of quantum defect, we obtained different curves some curves are upper lying curve, few curves are with some spikes and some are lower lying curves. In the graphs of radii we observed the exponential behavior and in the graphs of Rydberg energy it is observed that the increase of quantum number shows rapid increase in the energy after a certain level of the quantum number and then behavior is exponentially increased.

Table 1: Transition Probability as a Lower Level $1S^2$.

A(KI)	E(I)	E(K)	Lower level			Upper level			Radiative Life times
			Conf.	Term	J	Conf.	Term	J	
5.62E-01	0	956502	$1S^2$.	^{1}S	0	1s2s	^{3}S	1	1.045E-06
6.17E+02	0	983370	$1S^2$.	^{1}S	0	1s2p	^{3}P°	2	1.62E-03
1.22E+11	0	997454	$1S^2$.	^{1}S	0	1s2p	^{1}P°	1	
2.15E+02	0	1128300	$1S^2$.	^{1}S	0	1s3p	^{3}P°	2	4.65E-03
3.62E+10	0	1132390	$1S^2$.	^{1}S	0	1s3p	^{1}P°	1	
9.27E+01	0	1178174	$1S^2$.	^{1}S	0	1s4p	^{3}P°	2	1.08E-02
1.52E+10	0	1179830	$1S^2$.	^{1}S	0	1s4p	^{1}P°	1	
4.82E+01	0	1201060	$1S^2$.	^{1}S	0	1s5p	^{3}P°	2	2.07E-02
7.80E+09	0	1201894	$1S^2$.	^{1}S	0	1s5p	^{1}P°	1	
4.51E+09	0	1213931	$1S^2$.	^{1}S	0	1s6p	^{1}P°	1	2.217E-10
2.84E+09	0	1221135	$1S^2$.	^{1}S	0	1s7p	^{1}P°	1	3.521E-10
9.27E+05	0	1131462	$1S^2$.	^{1}S	0	1s3d	^{1}D	2	1.079E-06
5.22E+05	0	1179495	$1S^2$.	^{1}S	0	1s4d	^{1}D	2	1.916E-06
2.98E+05	0	1201800	$1S^2$.	^{1}S	0	1s5d	^{1}D	2	3.358E-06

Table 2: Calculated data for quantum defect, energy and radius of Be III (1sns $1S_0$)

Principal Quantum Number (n)	Quantum Defect	Energy of Be III	Radii	Principal Quantum Number (n)	Quantum Defect	Energy of Be III	Radii
2	0.051298	981178	3.46E-05	17	0.044276	1237821	0.00262
3	0.050821	1127705	7.92E-05	18	0.044245	1238193	0.002938
4	0.0485	1178005	0.000142	19	0.044218	1238508	0.003274
5	0.047065	1200997	0.000223	20	0.044195	1238777	0.003629
6	0.046194	1213395	0.000323	21	0.044176	1239008	0.004002
7	0.045638	1220835	0.000441	22	0.044159	1239208	0.004393
8	0.045265	1225649	0.000577	23	0.044144	1239382	0.004802
9	0.045004	1228941	0.000731	24	0.044131	1239536	0.00523
10	0.044815	1231291	0.000903	25	0.04412	1239671	0.005675
11	0.044673	1233028	0.001094	26	0.04411	1239791	0.006139
12	0.044565	1234347	0.001302	27	0.04410	1239897	0.006621
13	0.04448	1235372	0.00153	28	0.044092	1239993	0.007122
14	0.044413	1236186	0.001775	29	0.044085	1240079	0.00764
15	0.044358	1236841	0.002038	30	0.044079	1240156	0.008177
16	0.044313	1237377	0.00232				

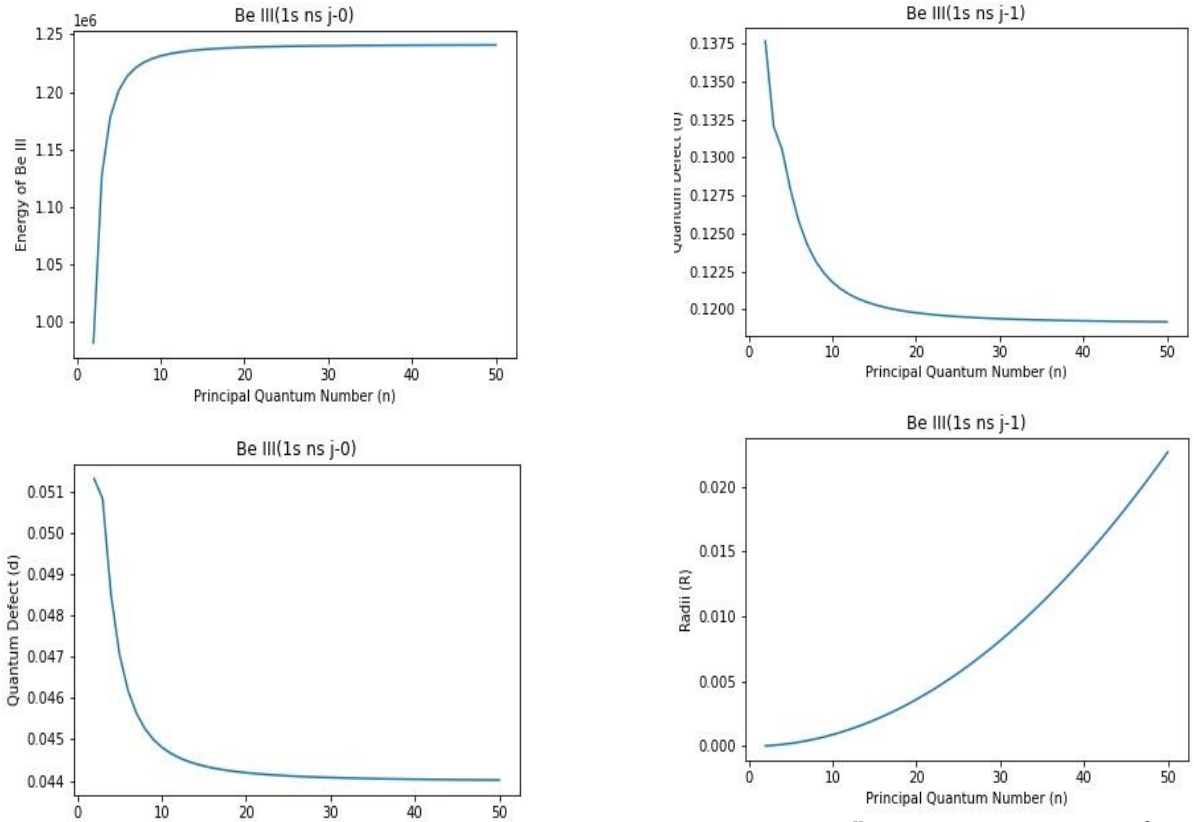
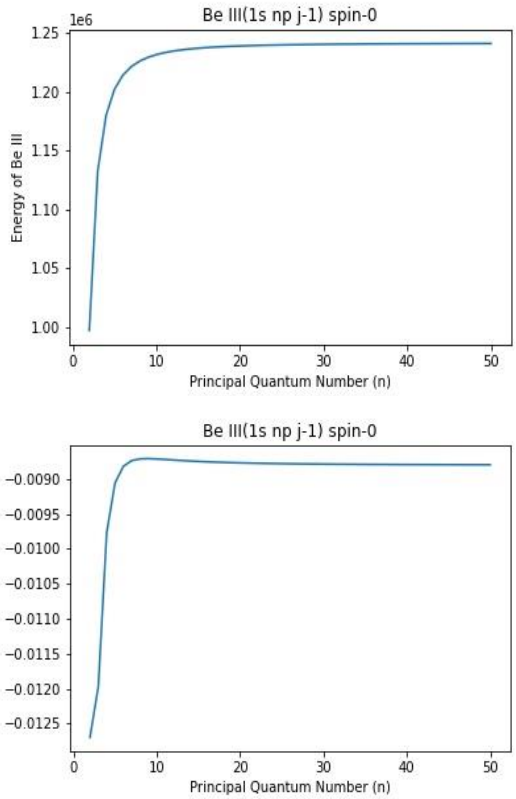


Figure 01: Rydberg Energy, Quantum Defect and Radii of Be-III (1sns $1S_0$ and $3S_1$)



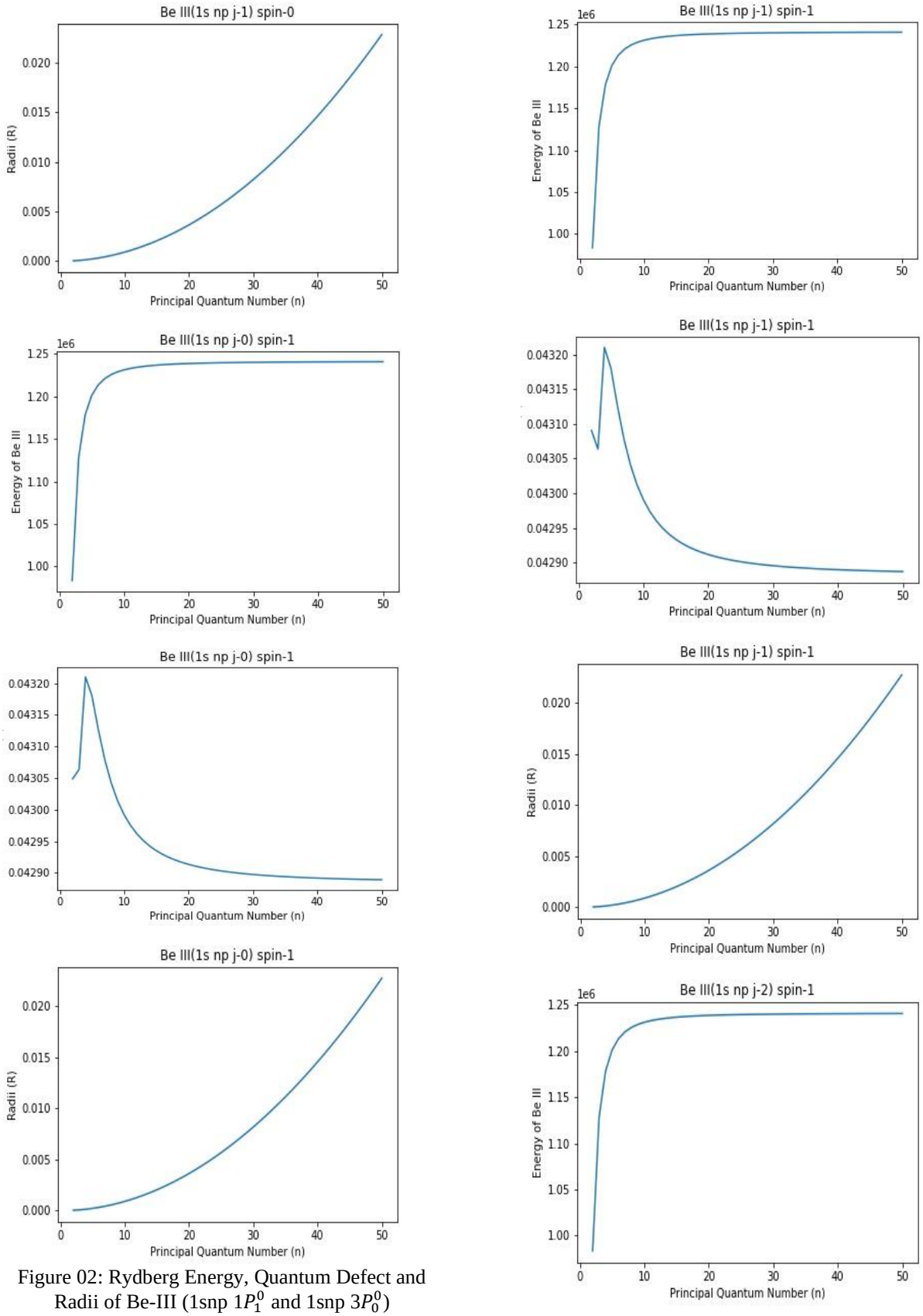


Figure 02: Rydberg Energy, Quantum Defect and Radii of Be-III (1snp $1P_1^0$ and 1snp $3P_0^0$)

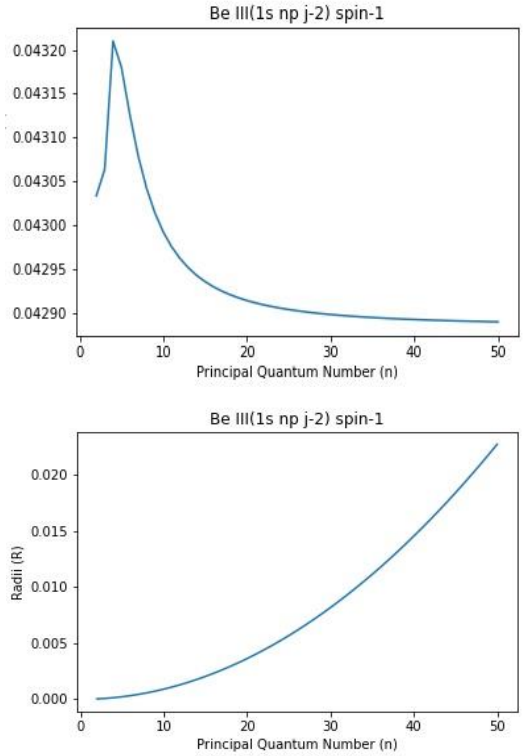
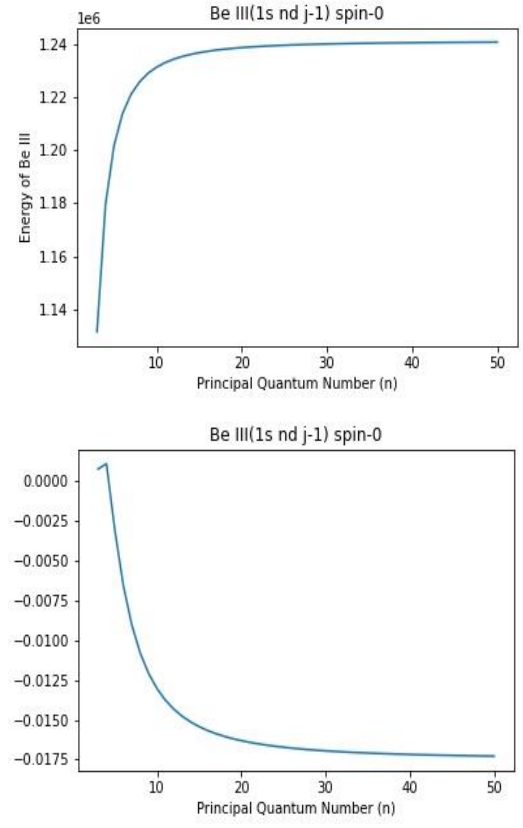
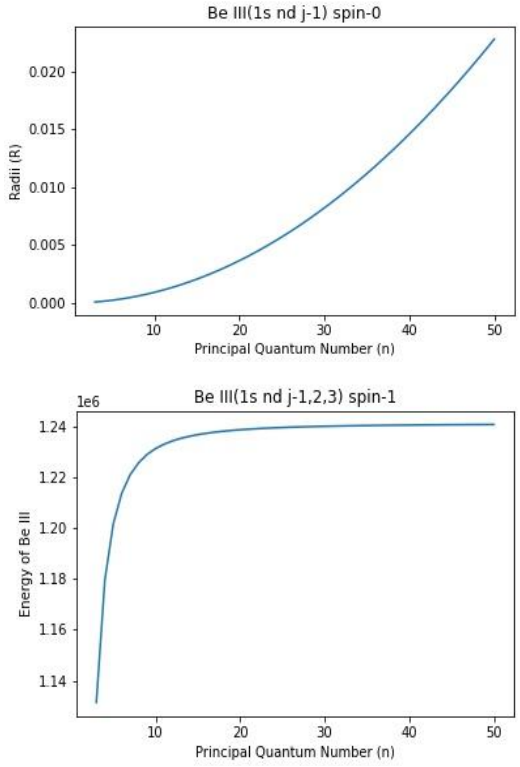


Figure 03: Rydberg Energy, Quantum Defect and Radii of Be-III (1snp $3P_1^0$ and 1snp $3P_2^0$)





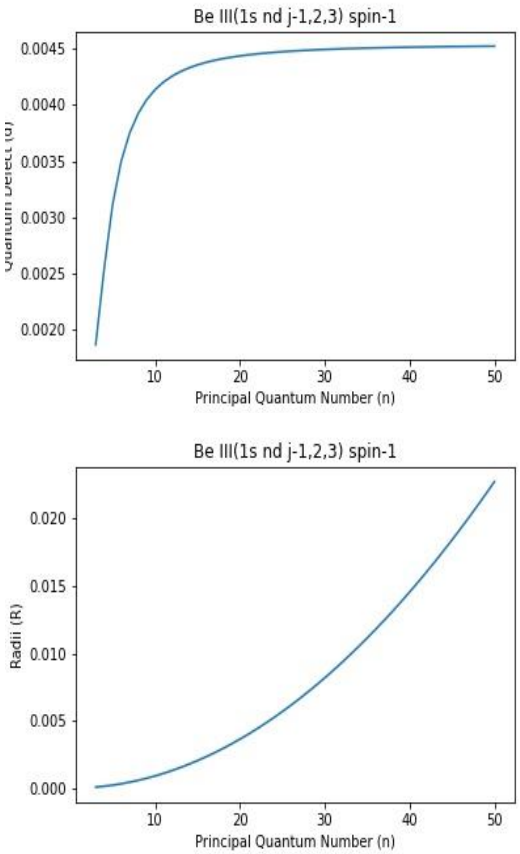
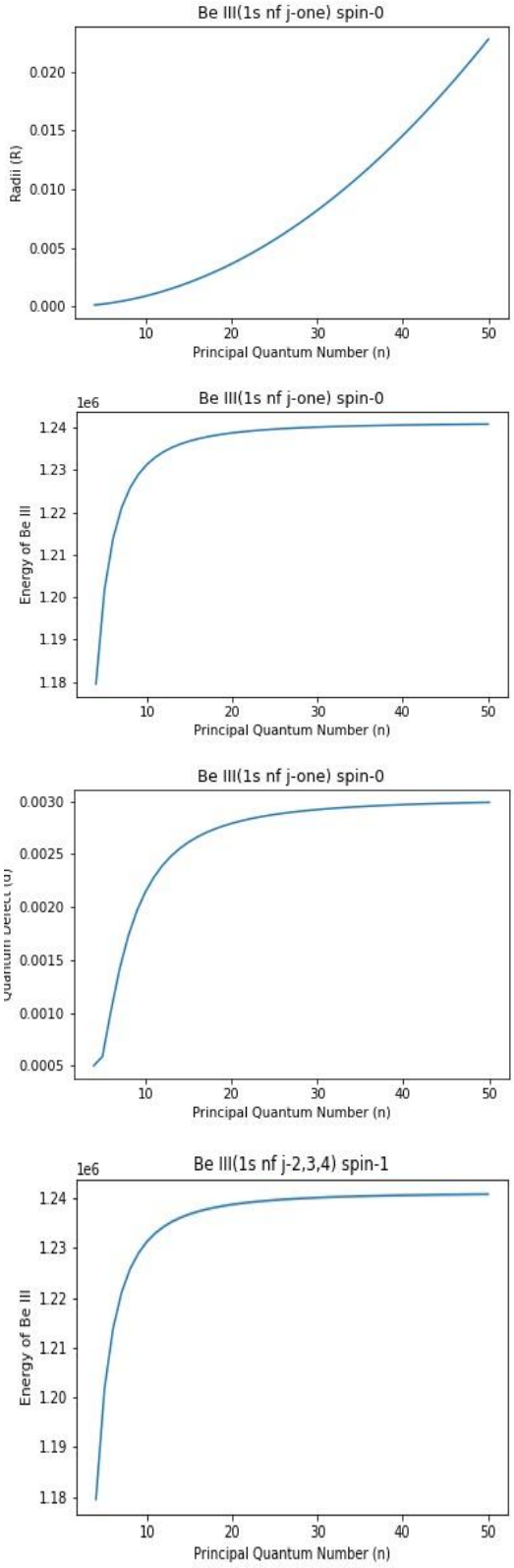


Figure 04: Rydberg Energy, Quantum Defect and Radii of Be-III (1snd $1D_2$ and 1snd $3D_{1,2,3}$)



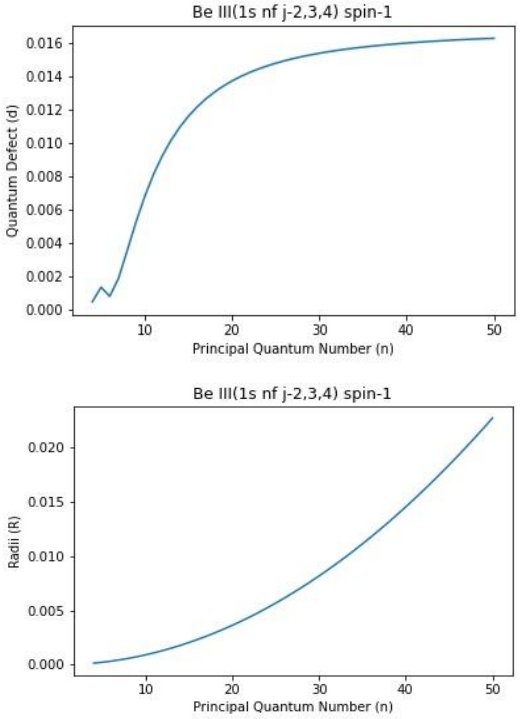


Figure 05: Rydberg Energy, Quantum Defect and Radii of Be-III (1snf $1F_3^0$ and 1snf $3F_{2,3,4}^0$)

IV. CONCLUSION

Beryllium is an important element from the astrophysical point of view. Many stars and astronomical objects emit lines of Be atom and its ions. The weakest bound electron potential theory was used in this study. The spectrum of Be III have been investigated, various properties of Be III (energy, quantum defect, radius, and lifetime) have been determined. Martin Formula was used to calculate energy and quantum defects of Rydberg levels. The lifetime of 157 Rydberg levels have also been calculated using necessary data obtained from NIST database. The Rydberg series 1sns $1S_0$, 1sns $3S_1$, 1snp $1P_1^0$, 1snp $3P_{0,1,2}^0$ J (spin-orbital coupling), 1snd $1D_2$, 1snd $3D_{1,2,3}$, 1snf $1F_3^0$ and 1snf $3F_{2,3,4}^0$ have been investigated and some of them are non-perturbed and other are perturbed. These data will be useful to find lifetime, Oscillator strength, line strength and transition probability in Be III. It can be also useful to found Purturber in different series.

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