

Transition Probabilities, Oscillator Strengths and Line Strengths Result From Radiative Transitions

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Doi: <https://doi.org/10.47011/16.5.9>

Received on: 30/01/2022;

Accepted on: 13/06/2022

Abstract: The single-electron approximation and quantum defect theory have been used to study the spectral properties of radiative transitions in beryllium ions (Be II). A total of 6386 transitions of Be II have been investigated. The lifetime of nS, nP, nD, and nF Rydberg states of Be II ($1s^2 nl$), for n up to 30, have been computed and compared with the available data. Most of the lifetimes are new. Transition probabilities, oscillator strengths, and line strengths of 6386 radiative transitions of Be II are being reported here. A Python program was developed to calculate the radial integral, and the same program was used to compute the corresponding expectation values $\langle r \rangle$, ensuring the validity of the results. This extensive study provides a substantial dataset on spectral properties of radiative transitions in Be II, which holds valuable applications in various spectroscopic contexts.

Keywords: Rydberg ion (atom), Radiative lifetimes, Oscillator strength, Transition probability, Rydberg energy, Beryllium ion.

1. Introduction

Transition probability and radiative lifetimes serve as fundamental characteristics of excited states in atoms, ions, and molecules, offering important information about atomic structure. Singly ionized alkaline-earth metal beryllium (Be-II) holds significance in theoretical and experimental atomic physics, astrophysics, space physics, and plasma. Beryllium has vast applications in gyroscopes, computer parts, instruments, nuclear work, and ceramic applications [1, 9]. While ample research has explored a range of spectroscopic characteristics of beryllium, there is a scarcity of literature specifically addressing transition probabilities. Bergström *et al.* employed the beam foil technique and measured some lifetimes of excited terms of Be I and Be II. These researchers used an isotope separator as an accelerator. The available energy at the separator, which ranged from 40 to 80 keV, was compatible with excitations of neutral and singly

ionized atoms [2]. T. Andersen *et al.* measured the lifetimes of excited states in neutral and ionic types of beryllium and boron employing the foil-excitation technique. An electromagnetic isotope separator was used to produce 60 - 400 keV ion beams. Wavelengths ranging from 1600 to 7000 Å were examined. They measured the lifetimes of 11 states of Be I, 09 of Be II, and 01 of Be III [3]. Lindgård and Nielsen derived the dipole transition probabilities, oscillator strengths, lifetimes, and branching ratios by employing the numerical Coulomb approximation for experimentally acknowledged and extrapolated states of alkali isoelectronic sequences [4]. J. Bromander *et al.* measured the lifetimes of five of the $n = 3$ terms in Be III. They studied the beam-foil spectra of Be for energies between 200 and 400 keV and wavelengths of 500 - 1200 Å. To find out the strong spectra of doubly excited Be II and Be III and to get the precise magnitude of short lifetimes, a heavy-ion accelerator of 600

keV was employed [5]. Chou used a relativistic many-body perturbation theory (MBPT) and calculated the transition rates for electric dipole transitions in Be-like ions. The worked-out transition rates were found in good concurrence with experiments for all ions [6]. Neng Wu Zheng *et al.* calculated the transition probabilities between *LS* multiples of Be and Mg ionic states. They employed the WBEPM for calculation. The effective charges Z^* and effective quantum numbers n^* and l^* were concluded through a coupled set of equations. Transition probabilities were estimated between highly excited states through modified hydrogen wavefunctions [7]. Fuhr and Wiese compiled the data of atomic transition probabilities for the spectra of beryllium and boron atoms and ions. They tabulated the data for about 1400 allowed and forbidden transitions by covering all ionization stages [8]. In 2016, Çelik *et al.* employed the WBEPM and quantum defect theory and calculated the lifetimes for singly ionized beryllium (Be II) [9]. Wang *et al.* employed the time-resolved laser-induced fluorescence technique to measure the radiative lifetimes of 05 levels in Be I. They further figured out transition probabilities and oscillator strengths for 90 Be I spectral lines [10]. This work aims to extend the known values of transition probabilities, oscillator strengths, and line strengths, which help to determine other spectroscopic characteristics, e.g., dipole polarizability.

2. Theory

In a multi-electron system, the outermost electron is supposed to be the most loosely bound (weakest bound) compared to the rest of the electronic cloud, thus, it can most easily be excited. If examined from an excitation aspect, the behavior of the weakest bound electron differs from its counterparts. Hence, the weakest bound electron can be dealt with alone. This notion simplifies a complex multi-electron problem to a single-electron problem [11]. This idea and quantum defect models were recently combined by Zheng *et al.* in the weakest bound electron potential model theory (WBEPM). The foundation of WBEPM rests on the proposal that in any system, the orbiting electrons may be grouped into the weakest and the non-weakest bound electrons [12-16]. The weakest bound electron is supposed to be in a field created by the nucleus and inner core electrons. When

excited to a higher energy level, the weakest electron moves in an enlarged orbit for a longer period. Consequently, the coupling between core and weakest bound electrons diminishes [17]. The single-electron Hamiltonian and corresponding nonrelativistic Schrödinger equation for the weakest bound electron i are given below:

$$H_i = -\frac{1}{2} + \nabla_i^2 + V(r_i) \quad (1)$$

$$\left[-\frac{1}{2} + \nabla_i^2 + V(r_i)\right] \psi_i = \varepsilon_i \psi_i \quad (2)$$

Using the polar coordinates and separating the angular part, we get the radial part as

$$\frac{d^2 R}{dr^2} + \frac{2}{r} \frac{dR}{dr} + 2 \left(E - \frac{A}{r_i} - \frac{B}{r_i^2} - \frac{l(l+1)}{r_i^2} \right) = 0 \quad (3)$$

Here, $A/r_i - B/r_i^2 = V(r_i)$ is the potential observed by the weakest bound (WB) electrons. $A = -z^*$ is the effective nuclear charge where r_i is the distance between the WB electron i and the nucleus.

$B = \frac{d(d+1)+2dl}{2}$ wherein the factor d has been introduced due to quantum defects. It is the modification of integral values of n and l into non-integral values n^* and l^* . Hence Eq. (3) becomes:

$$\frac{d^2 R}{dr^2} + \frac{2}{r} \frac{dR}{dr} + 2 \left(E + \frac{Z^*}{r_i} - \frac{l^*(l^*+1)}{r_i^2} \right) = 0 \quad (4)$$

Here, $2B + l(l+1) = l^*(l^*+1)$ and $l^* = l - \delta_n$, $n^* = n - \delta_n$, are effective orbital- and principal-quantum numbers, respectively, whereas, δ_n is the quantum defect and is given as a function of n :

$$\delta_n = a + \frac{b}{(n-\delta_o)^2} + \frac{c}{(n-\delta_o)^4} + \frac{d}{(n-\delta_o)^6} \quad (5)$$

Here δ_o 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 weakest bound electron is given as

$$E = -\frac{Z^{*2}}{2n^{*2}} = -\frac{Z^{*2}}{2(n-\delta_n)^2} \quad (6)$$

The solution of Eq. (4) gives the radial wave function R as

$$R = C \exp\left(-\frac{Z^* r}{n^*}\right) r^{l^*} L_{n^*-l^*-1}^{2l^*+1}\left(\frac{2Z^* r}{n^*}\right) \quad (7)$$

$$\text{where } C = \left(\frac{2Z^*}{n^*}\right)^{l^*+\frac{3}{2}} \sqrt{\frac{(n^*-l^*-1)!}{2n^* \Gamma(n^*+l^*+1)}}$$

The transition probability A_{fi} of a transition for spontaneous emission between levels (n_f, l_f) & (n_i, l_i) , is given as

$$A_{fi} = 20261 \times 10^{-6} \frac{(E_f - E_i)^3}{2l_i + 1} S \quad (8)$$

Where, $E_f > E_i$ and are the energies of upper and lower states, respectively. S is the electric dipole line strength. Since the LS coupling dominates in lighter atoms, thus the line strength may be:

$$S_{LS} = [J_f, J_i, L_f, L_i] \left(\begin{Bmatrix} L_f & S & J_f \\ J_i & 1 & L_i \end{Bmatrix} \begin{Bmatrix} L_f & l_f & L_c \\ 1 & L_i & l_i \end{Bmatrix} P_{l_i l_f}^{(1)} \right)^2 \quad (9)$$

The terms contain two 6J symbols in brackets and a matrix element $P_{l_i l_f}^{(1)}$, which is given as

$$P_{l_i l_f}^{(1)} = l_{>} \langle n_i, l_i | r | n_f, l_f \rangle = l_{>} \int_0^\infty r^3 R_{n_i l_i} R_{n_f l_f} dr \quad (10)$$

The lifetime of a state is the sum of reciprocals of transition probabilities of all possible transitions from the state. The following expression gives the lifetime:

$$\tau_J = \sum_{J'} \frac{1}{A_{JJ'}} \quad (11)$$

3. Results and Discussion

Numerical calculations of lifetimes, transition probabilities, oscillator strengths, etc., have been carried out via many electron self-consistent methods and single-electron approximations. While most of the calculations so far have been limited to $n < 11$, in this study, we extended the calculations up to $n < 31$. Hydrogen-like atoms or ions were considered within a single electron approximation, and the wavefunctions, expressed in terms of Laguerre polynomials with modified principal and orbital quantum numbers, were utilized. Quantum defects, determining the modification in quantum numbers, were calculated using quantum defect theory. The wavefunctions for ns, np, nd, and nf states up to $n = 30$ were calculated using Laguerre polynomials given in Eq. (7). Electric dipole matrix elements were computed using these wavefunctions in Eq. (10), and a Python code was developed for the integration. The radial integral [Eq. (10)] was calculated by Python code generated in this study. The reliability of

codes is confirmed by calculating the expectation values $\langle r \rangle$ for ns, np, nd, and nf orbits by Eq. (12).

$$\langle r \rangle = \frac{3n^{*2} - l^*(l^* + 1)}{2Z^*} \quad (12)$$

We used $Z^* = 2$ to calculate quantum defects and Rydberg energies, and the resulting values were compared with the literature [18]. Glukhov *et al.* [18] have also used $Z = 2$ for the determination of quantum defects. The values of the electric dipole matrix elements were used in Eq. (9) to calculate line strengths, which, in turn, were employed in Eq. (8) to calculate transition probabilities. Finally, lifetimes for nS, nP, nD, and nF states were computed using Eq. (11), totaling 112 lifetimes for 6386 radiative transitions in Be II.

Table 1 presents the lifetimes of 112 states of Be II up to $n = 30$. The multiplicity due to spin-orbit coupling makes no difference, the counterparts of each state have the same values of lifetimes, and it is immaterial to mention the J values of each state. Therefore, only one element from each multiplicity is shown in the table. The lifetimes are compared with the corresponding works of [18, 19]. The lifetime results of Theodosiou [19] and Glukhov *et al.* [18] are in good agreement with the experimental results [3,5]. The results of this study are in excellent agreement with the results of Çelik *et al.* [9], Theodosiou, Glukhov *et al.* [18], and [30, 31], therefore, Table 1 shows only lifetimes calculated by Glukhov *et al.* [18] for comparison. Both Theodosiou and Glukhov *et al.* calculated lifetimes up to $n < 11$. In this work, the nS, nP, nD, and nF lifetimes are calculated up to $n < 31$.

Zheng *et al.* [7] calculated transition probabilities of one hundred transitions of Be II using the weakest bound electron potential model. The results of our calculations are in good agreement with the corresponding findings published by Zheng *et al.* [7]. Table 2 shows the transition probabilities, oscillator strengths, and line strengths for transitions listed on the NIST site [20]. There are almost 6386 transition probabilities calculated in this work, with the majority being new and presented in a supplementary table accompanying the manuscript. In most cases, the deviation from known values is less than 1%, with some cases below 5%, and only a few instances exhibit variations exceeding 5%. Figures 1 and 2

compare calculated values of transition probabilities and oscillator strengths for the transitions nP to $2S$ state and the corresponding values taken from NIST data, encompassing n

lines between 1 and 9. These figures illustrate a high level of agreement between calculated values and those taken from the NIST site.

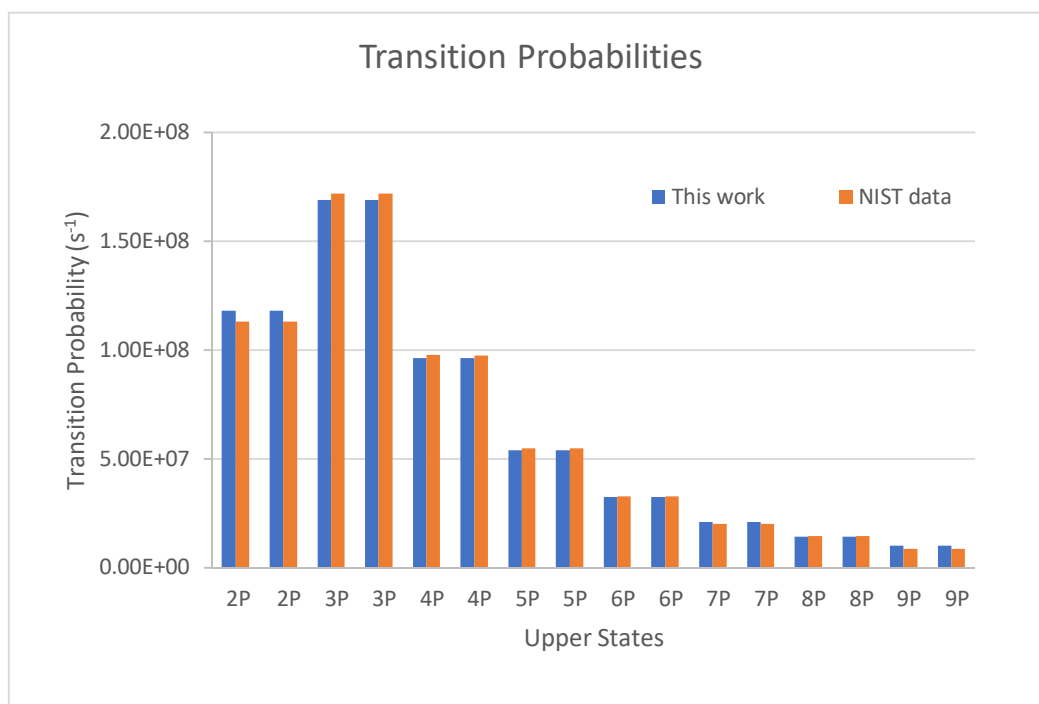


FIG. 1. Comparison of transition probabilities in NIST data and calculated in this work for the transition from nP to $2S$ state.

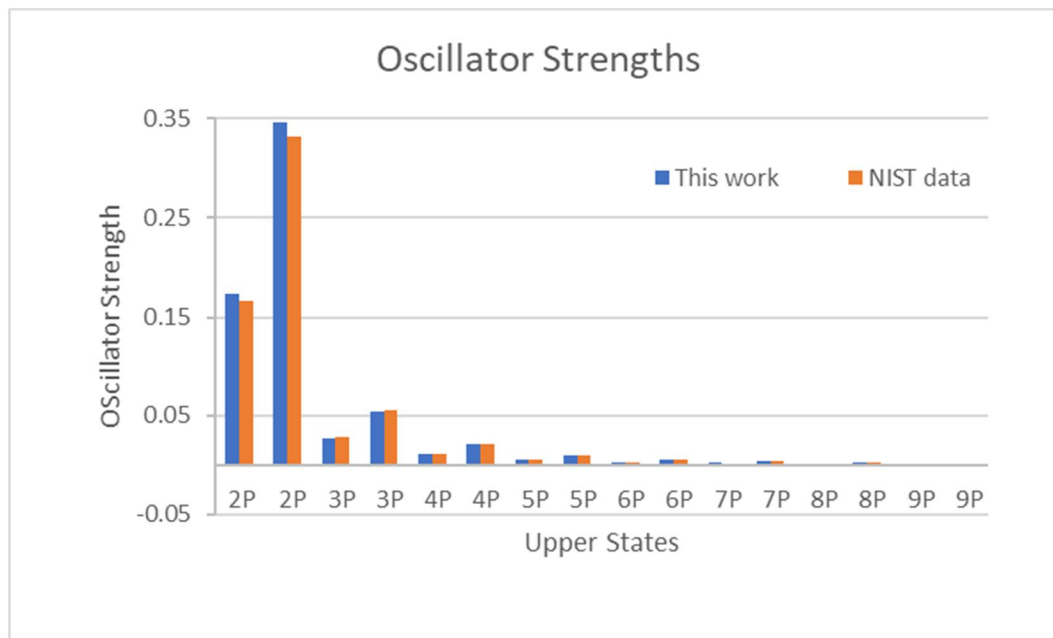


FIG. 2. Comparison of oscillator strengths in NIST data and calculated in this work for the transition from nP to $2S$ state.

TABLE 1. Radiative Lifetimes of s, p, d, and $f(l \pm s)$ sequence of Rydberg levels compared with previously published data for Be II.

Radiative Lifetimes τ (nSec)											
Confi	$(2s+l) L_j$	This	CAHS	FMP	WBEPMT	QDT	Experimental	RMBT	Kazakov	Kurucz	Other Results
g.		Work	[19]	[18]	[9]	[9]	Results	[29]	[30]	[31]	
	$3s \quad ^2S_{1/2}$	2.46	2.473	2.461	2.46	2.46	$3.3(4)^c, 2.0(2)^d, 2.3(3)^f$	2.451(1)	2.5	2.545	$2.51^a, 2.37^c, 2.38^g$
	$4s \quad ^2S_{1/2}$	4.19	4.196	4.199	4.24	4.2	$4.4(3)^c, 4.9(3)^d, 5.0(3)^f, 4.2(3)^i$	4.174(1)	4.3	4.486	4.254^a
	$5s \quad ^2S_{1/2}$	7.22	7.213	7.236	7.35	7.24		7.914(2)	7.3	7.519	
	$6s \quad ^2S_{1/2}$	11.73	11.7	11.76	12	11.8		11.673(2)	12	12.21	
	$7s \quad ^2S_{1/2}$	17.99	18.02	18.02	18.4	18		17.918(4)	18.5	18.622	
	$8s \quad ^2S_{1/2}$	26.29	26.22	26.34	25.9	26.4		26.17(1)	26.5	27.174	
	$9s \quad ^2S_{1/2}$	36.93	36.81	36.99	37.9	37		36.78(2)	37.5	38.023	
	$10s \quad ^2S_{1/2}$	50.19	50.02	50.27	51.5	50.3		49.89(7)	51	51.546	
	$11s \quad ^2S_{1/2}$	66.37	66.14								
	$12s \quad ^2S_{1/2}$	85.78	85.44								
	$13s \quad ^2S_{1/2}$	108.70									
	$14s \quad ^2S_{1/2}$	135.44									
	$15s \quad ^2S_{1/2}$	166.30									
1	$16s \quad ^2S_{1/2}$	201.57									
	$17s \quad ^2S_{1/2}$	241.56									
	$18s \quad ^2S_{1/2}$	286.55									
	$19s \quad ^2S_{1/2}$	336.86									
	$20s \quad ^2S_{1/2}$	392.77									
	$21s \quad ^2S_{1/2}$	454.59									
	$22s \quad ^2S_{1/2}$	522.62									
	$23s \quad ^2S_{1/2}$	597.15									
	$24s \quad ^2S_{1/2}$	678.48									
	$25s \quad ^2S_{1/2}$	766.92									
	$26s \quad ^2S_{1/2}$	862.76									
	$27s \quad ^2S_{1/2}$	966.29									
	$28s \quad ^2S_{1/2}$	1077.83									
	$29s \quad ^2S_{1/2}$	1197.63									
	$30s \quad ^2S_{1/2}$	1326.03									

Radiative Lifetimes τ (nSec)											
Confi g.	$(2s+1) L_j$	This Work	CAHS [19]	FMP [18]	WBEPMT [9]	QDT [9]	Experimental Results	RMBT [29]	Kazakov [30]	Kurucz [31]	Other Results
2	$2p \ ^2P^o_{1\pm 1/2}$	8.48	8.93	8.504	8.64	8.5	8.1(4) ^c , 9.5(2) ^f , 8.7(2) ⁱ	8.85(2)	8.9	8.621	8.939 ^a , 8.62 ^e , 8.63 ^g , 8.85 ^j
	$3p \ ^2P^o_{1\pm 1/2}$	5.51	5.431	5.522	5.18	5.52	6.7(8) ⁱ	5.417(2)	5.6	4.149	5.615 ^a , 5.58 ^e , 5.55 ^g
	$4p \ ^2P^o_{1\pm 1/2}$	8.21	8.03	8.232	8.07	8.23	8.1(8) ^b , 8.5(9) ⁱ	8.086(1)	8.3	6.211	8.312 ^a
	$5p \ ^2P^o_{1\pm 1/2}$	13.12	12.76	13.15	13.1	13.2		12.918(4)	13.5	9.901	
	$6p \ ^2P^o_{1\pm 1/2}$	20.34	19.71	20.39	20.6	20.4		20.05(1)	20.5	15.432	
	$7p \ ^2P^o_{1\pm 1/2}$	30.22	29.19	30.29	30.8	30.3		29.78(2)	30.5	22.936	
	$8p \ ^2P^o_{1\pm 1/2}$	43.17	41.57	43.25	44.1	44.3		42.66(4)	43.5	32.68	
	$9p \ ^2P^o_{1\pm 1/2}$	59.58	57.25	59.69	61.1	59.1		58.86(7)	60.1	45.045	
	$10p \ ^2P^o_{1\pm 1/2}$	79.90	76.66	80.03	82.2	80.1		78.6(2)	80.5	60.606	
	$11p \ ^2P^o_{1\pm 1/2}$	104.53	100.1								
	$12p \ ^2P^o_{1\pm 1/2}$	133.91	128.1								
	$13p \ ^2P^o_{1\pm 1/2}$	168.46									
	$14p \ ^2P^o_{1\pm 1/2}$	208.62									
	$15p \ ^2P^o_{1\pm 1/2}$	254.80									
	$16p \ ^2P^o_{1\pm 1/2}$	307.44									
	$17p \ ^2P^o_{1\pm 1/2}$	366.97									
	$18p \ ^2P^o_{1\pm 1/2}$	433.82									
	$19p \ ^2P^o_{1\pm 1/2}$	508.41									
	$20p \ ^2P^o_{1\pm 1/2}$	591.18									
	$21p \ ^2P^o_{1\pm 1/2}$	682.57									
$22p \ ^2P^o_{1\pm 1/2}$	782.99										
$23p \ ^2P^o_{1\pm 1/2}$	892.88										
$24p \ ^2P^o_{1\pm 1/2}$	1012.68										
$25p \ ^2P^o_{1\pm 1/2}$	1142.80										
$26p \ ^2P^o_{1\pm 1/2}$	1283.70										
$27p \ ^2P^o_{1\pm 1/2}$	1435.78										
$28p \ ^2P^o_{1\pm 1/2}$	1599.50										
$29p \ ^2P^o_{1\pm 1/2}$	1775.26										
$30p \ ^2P^o_{1\pm 1/2}$	1963.34										

Transition Probabilities, Oscillator Strengths and Line Strengths Result From Radiative Transitions

Radiative Lifetimes τ (nSec)												
Confi	$(2s+1) L_j$	This	CAHS	FMP	WBEPMT	QDT	Experimental	RMBT	Kazakov	Kurucz	Other Results	
g.		Work	[19]	[18]	[9]	[9]	Results	[29]	[30]	[31]		
	$3d \ ^2D_{2\pm 1/2}$	0.86	0.911	0.862	0.892	0.862	$0.83(8)^d, 0.92(26)^f, 1.0(1)^i$	0.901(1)	0.9045	0.893	0.911 ^a	
	$4d \ ^2D_{2\pm 1/2}$	1.99	2.081	1.991	2.02	1.99	$2.3(2)^c, 2.12(9)^f, 2.30(9)^f$ $2.4(2)^i$	2.066(1)	2.1	2.075	2.069 ^a	
	$5d \ ^2D_{2\pm 1/2}$	3.81	3.971	3.817	3.83	3.82	$5.1(3)^c, 3.5(4)^i$	3.938(2)	3.9	3.984	3.940 ^a	
	$6d \ ^2D_{2\pm 1/2}$	6.49	6.754	6.507	6.501	6.51	$8.0(8)^c, 7.3(8)^i$	6.700(2)	6.7	6.757	6.688 ^a	
	$7d \ ^2D_{2\pm 1/2}$	10.21	10.61	10.23	10.2	10.2		10.518(4)	10.5	10.65		
	$8d \ ^2D_{2\pm 1/2}$	15.13	15.71	15.16	15.1	15.2		15.58(1)	15.5	15.773		
	$9d \ ^2D_{2\pm 1/2}$	21.41	22.22	21.46	21.3	21.5		22.01(1)	22	22.321		
	$10d \ ^2D_{2\pm 1/2}$	29.24	30.33									
	$11d \ ^2D_{2\pm 1/2}$	38.78	40.22									
	$12d \ ^2D_{2\pm 1/2}$	50.19	52.04									
	$13d \ ^2D_{2\pm 1/2}$	63.65										
	$14d \ ^2D_{2\pm 1/2}$	79.34										
	$15d \ ^2D_{2\pm 1/2}$	97.41										
3	$16d \ ^2D_{2\pm 1/2}$	118.04										
	$17d \ ^2D_{2\pm 1/2}$	141.39										
	$18d \ ^2D_{2\pm 1/2}$	167.65										
	$19d \ ^2D_{2\pm 1/2}$	196.97										
	$20d \ ^2D_{2\pm 1/2}$	229.53										
	$21d \ ^2D_{2\pm 1/2}$	265.50										
	$22d \ ^2D_{2\pm 1/2}$	305.05										
	$23d \ ^2D_{2\pm 1/2}$	348.34										
	$24d \ ^2D_{2\pm 1/2}$	395.55										
	$25d \ ^2D_{2\pm 1/2}$	446.85										
	$26d \ ^2D_{2\pm 1/2}$	502.41										
	$27d \ ^2D_{2\pm 1/2}$	562.39										
	$28d \ ^2D_{2\pm 1/2}$	626.98										
	$29d \ ^2D_{2\pm 1/2}$	696.32										
	$30d \ ^2D_{2\pm 1/2}$	770.55										

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Confi g.	$(2s+1) L_j$	This Work	CAHS [19]	FMP [18]	WBEPMT [9]	QDT [9]	Experimental Results	RMBT [29]	Kazakov [30]	Kurucz [31]	Other Results	
4	$4f$	${}^2F_{3\pm 1/2}$	4.50	4.52	4.51	4.51	4.51	7.0(4) ^c , 4.9(2) ^f ,	4.525(1)	4.522	4.523	4.523 ^a
	$5f$	${}^2F_{3\pm 1/2}$	8.71	8.739	8.722	8.71	8.72	9.7(7) ^c , 9.0(8) ⁱ	8.734(1)	8.739	8.737	8.737 ^a
	$6f$	${}^2F_{3\pm 1/2}$	14.92	14.93	14.91	14.9	14.9	9.3(10) ⁱ	14.948(6)	14.93	14.93	14.93 ^a
	$7f$	${}^2F_{3\pm 1/2}$	23.55	23.49	23.45	23.4	23.5		23.60(1)	23.49		
	$8f$	${}^2F_{3\pm 1/2}$	34.97	34.77	34.72	34.7	34.3		35.03(1)	34.77		
	$9f$	${}^2F_{3\pm 1/2}$	49.59	49.48	49.13	49.1	49.1		49.73(2)	49.18	49.261	
	$10f$	${}^2F_{3\pm 1/2}$	67.80	67.08		66.9	66.9				67.114	
	$11f$	${}^2F_{3\pm 1/2}$	90.00	88.85								
	$12f$	${}^2F_{3\pm 1/2}$	116.58	114.9								
	$13f$	${}^2F_{3\pm 1/2}$	147.93									
	$14f$	${}^2F_{3\pm 1/2}$	184.46									
	$15f$	${}^2F_{3\pm 1/2}$	226.56									
	$16f$	${}^2F_{3\pm 1/2}$	274.62									
	$17f$	${}^2F_{3\pm 1/2}$	329.05									
	$18f$	${}^2F_{3\pm 1/2}$	390.23									
	$19f$	${}^2F_{3\pm 1/2}$	458.56									
	$20f$	${}^2F_{3\pm 1/2}$	534.44									
	$21f$	${}^2F_{3\pm 1/2}$	618.27									
	$22f$	${}^2F_{3\pm 1/2}$	710.43									
	$23f$	${}^2F_{3\pm 1/2}$	811.34									
$24f$	${}^2F_{3\pm 1/2}$	921.37										
$25f$	${}^2F_{3\pm 1/2}$	1040.94										
$26f$	${}^2F_{3\pm 1/2}$	1170.42										
$27f$	${}^2F_{3\pm 1/2}$	1310.23										
$28f$	${}^2F_{3\pm 1/2}$	1460.73										
$29f$	${}^2F_{3\pm 1/2}$	1622.35										
$30f$	${}^2F_{3\pm 1/2}$	1795.48										

^a ref. [21], ^b ref. [23], ^c ref. [3], ^d ref. [22], ^e ref. [24], ^f ref. [25], ^g ref. [26], ⁱ ref. [27], ^j ref. [28].

TABLE 2. List of transition probabilities, oscillator strengths, and line strengths compared with NIST data

Transition	Transition Probability (s ⁻¹)			Oscillator Strength			Line Strength (a.u.)		
	This work	NIST	% Error	This work	NIST	% Error	This work	NIST	% Error
2S ---> 2P	1.18E+08	1.13E+08	4.46630	0.17299	0.16596	4.23575	3.56656	3.42230	4.21527
2S --> 2P	1.18E+08	1.13E+08	4.40154	0.34598	0.33198	4.21691	7.13312	6.84450	4.21679
2S ---> 3P	1.69E+08	1.72E+08	1.79255	0.02713	0.02768	1.98565	0.18511	0.18890	2.00597
2S ---> 3P	1.69E+08	1.72E+08	1.95232	0.05423	0.05540	2.10590	0.37003	0.37800	2.10925
2S ---> 4P	9.63E+07	9.79E+07	1.59749	0.01022	0.01040	1.72409	0.05666	0.05770	1.80067
2S ---> 4P	9.63E+07	9.76E+07	1.32908	0.02043	0.02070	1.28474	0.11328	0.11500	1.49511
2S ---> 5P	5.41E+07	5.50E+07	1.68348	0.00486	0.00496	1.92708	0.02483	0.02530	1.85025
2S ---> 5P	5.41E+07	5.50E+07	1.71442	0.00973	0.00991	1.85966	0.04965	0.05060	1.88212
2S ---> 6P	3.26E+07	3.30E+07	1.22905	0.00270	0.00274	1.58319	0.01320	0.01340	1.48292
2S ---> 6P	3.26E+07	3.30E+07	1.24155	0.00539	0.00547	1.41590	0.02640	0.02680	1.49562
2S ---> 7P	2.10E+07	2.03E+07	3.32291	0.00165	0.00160	3.30564	0.00790	0.00764	3.36760
2S ---> 7P	2.10E+07	2.03E+07	3.32879	0.00331	0.00320	3.31157	0.01580	0.01530	3.23843
2S ---> 8P	1.42E+07	1.47E+07	3.18341	0.00109	0.00112	2.90421	0.00512	0.00529	3.28439
2S ---> 8P	1.42E+07	1.47E+07	3.16361	0.00218	0.00225	3.31587	0.01023	0.01060	3.44697
2S ---> 9P	1.01E+07	8.76E+06	15.03572	0.00075	0.00066	14.78235	0.00351	0.00306	14.74375
2S ---> 9P	1.01E+07	8.75E+06	15.20381	0.00151	0.00131	15.16959	0.00702	0.00611	14.96831
2P ---> 3S	1.36E+08	1.36E+08	0.27902	0.06408	0.06438	0.45934	0.74949	0.75290	0.45356
2P ---> 3S	2.71E+08	2.72E+08	0.27902	0.06408	0.06438	0.45934	1.49897	1.50600	0.46678
2P---> 3D	9.68E+08	9.22E+08	5.02624	1.29582	0.63200	105.03481	6.59918	6.29300	4.86542
2P---> 3D	1.94E+08	1.84E+08	5.04903	0.13358	0.06321	111.32732	1.31984	1.25900	4.83211
2P---> 3D	1.16E+09	1.11E+09	5.03087	0.59644	0.56890	4.84075	11.87833	11.33000	4.83967
2P ---> 4S	4.74E+07	4.84E+07	2.07925	0.01016	0.01039	2.22786	0.08007	0.08191	2.24436
2P ---> 4S	9.47E+07	9.67E+07	2.04887	0.01016	0.01039	2.22786	0.16014	0.16380	2.23243
2P---> 4D	3.25E+08	3.14E+08	3.59168	0.12719	0.12300	3.40865	0.95721	0.92500	3.48255
2P---> 4D	6.51E+07	6.27E+07	3.75689	0.01272	0.01230	3.40865	0.19144	0.18500	3.48255
2P---> 4D	3.90E+08	3.75E+08	4.09202	0.11448	0.11000	4.06924	1.72302	1.66000	3.79649
2P---> 5S	2.23E+07	2.26E+07	1.27329	0.00367	0.00372	1.38246	0.02532	0.02570	1.48573
2P ---> 5S	4.46E+07	4.52E+07	1.27329	0.00367	0.00372	1.38246	0.05064	0.05140	1.48573
2P---> 5D	1.51E+08	1.46E+08	3.71325	0.04779	0.04630	3.22637	0.32315	0.31300	3.24350
2P---> 5D	3.03E+07	2.93E+07	3.35928	0.00478	0.00463	3.22637	0.06463	0.06260	3.24350
2P---> 5D	1.82E+08	1.76E+08	3.24568	0.04302	0.04160	3.40367	0.58169	0.56300	3.32033

Transition	Transition Probability (s^{-1})			Oscillator Strength			Line Strength (a.u.)		
	This work	NIST	% Error	This work	NIST	% Error	This work	NIST	% Error
2P---> 6S	1.23E+07	1.24E+07	0.73980	0.00178	0.00181	1.46383	0.01156	0.01170	1.23905
2P ---> 6S	2.46E+07	2.48E+07	0.73980	0.00178	0.00180	0.91641	0.02311	0.02330	0.81518
2P---> 6D	8.34E+07	8.08E+07	3.22919	0.02365	0.02290	3.25825	0.15152	0.14700	3.07639
2P---> 6D	1.67E+07	1.62E+07	2.97430	0.00236	0.00229	3.25825	0.03030	0.02940	3.07639
2P---> 6D	1.00E+08	9.71E+07	3.08035	0.02128	0.02070	2.80930	0.27274	0.26500	2.92081
2P---> 7S	7.51E+06	7.60E+06	1.13924	0.00101	0.00103	1.52560	0.00634	0.00643	1.35632
2P---> 7S	1.50E+07	1.53E+07	1.78539	0.00101	0.00103	1.52560	0.01269	0.01290	1.66219
2P---> 7D	6.12E+07	5.95E+07	2.90241	0.01223	0.01190	2.81351	0.15201	0.14800	2.70823
2P---> 7D	5.10E+07	4.95E+07	3.08070	0.01359	0.01320	2.99155	0.08445	0.08210	2.86604
2P---> 7D	1.02E+07	9.89E+06	3.18492	0.00136	0.00132	2.99155	0.01689	0.01640	2.99148
2P---> 8D	4.03E+07	3.91E+07	2.97413	0.00774	0.00753	2.73303	0.09424	0.09170	2.77284
2P---> 8D	3.36E+07	3.26E+07	2.93129	0.00860	0.00837	2.70179	0.05236	0.05100	2.67050
2P---> 8D	6.71E+06	6.52E+06	2.93129	0.00086	0.00084	2.70179	0.01047	0.01020	2.67050
2P---> 9D	2.33E+07	2.28E+07	2.07489	0.00581	0.00571	1.68461	0.03490	0.03430	1.75580
2P---> 9D	4.65E+06	4.57E+06	1.85153	0.00058	0.00057	1.68461	0.00698	0.00686	1.75580
2P---> 9D	2.79E+07	2.74E+07	1.91212	0.00522	0.00513	1.84937	0.06282	0.06170	1.80819
3S---> 3P	1.28E+07	1.26E+07	1.65085	0.28071	0.27670	1.44915	22.36679	22.05000	1.43671
3S---> 3P	1.28E+07	1.26E+07	1.64285	0.56156	0.55350	1.45599	44.73425	44.09000	1.46121
3S---> 4P	1.43E+07	1.41E+07	1.34336	0.02294	0.02270	1.07893	0.49486	0.48900	1.19796
3S---> 4P	1.43E+07	1.41E+07	1.27587	0.04586	0.04540	1.00625	0.98898	0.97900	1.01923
3S---> 5P	1.07E+07	1.06E+07	1.28939	0.00968	0.00959	0.94745	0.15646	0.15500	0.93981
3S---> 5P	1.07E+07	1.06E+07	1.23747	0.01935	0.01910	1.31616	0.31274	0.30900	1.21136
3P---> 3D	6.58E+04	6.58E+04	0.04534	0.08095	0.08113	0.22119	34.18412	34.26000	0.22149
3P---> 4S	3.22E+07	3.23E+07	0.55490	0.13376	0.13470	0.69857	4.64281	4.67700	0.73099
3P---> 4D	9.40E+07	9.09E+07	3.44070	0.53546	0.51900	3.17095	15.37810	14.90000	3.20872
3P---> 5S	1.37E+07	1.39E+07	1.18300	0.02161	0.02190	1.31165	0.46142	0.46700	1.19407
3P---> 5D	4.81E+07	4.65E+07	3.45453	0.13371	0.13000	2.85722	2.68293	2.60000	3.18956
3P ---> 6S	7.32E+06	7.37E+06	0.66040	0.00798	0.00805	0.90771	0.14172	0.14300	0.89838
3P---> 6D	2.73E+07	2.65E+07	2.86291	0.05595	0.05440	2.85220	0.96474	0.93800	2.85056
3P---> 7S	4.39E+06	4.43E+06	0.85736	0.00396	0.00401	1.16488	0.06408	0.06480	1.11407
3P---> 7D	1.69E+07	1.64E+07	2.98463	0.02946	0.02870	2.64609	0.46824	0.45600	2.68490
3P---> 8D	1.12E+07	1.09E+07	2.61524	0.01767	0.01720	2.73903	0.26731	0.26000	2.81263

Transition Probabilities, Oscillator Strengths and Line Strengths Result From Radiative Transitions

Transition	Transition Probability (s^{-1})			Oscillator Strength			Line Strength (a.u.)		
	This work	NIST	% Error	This work	NIST	% Error	This work	NIST	% Error
3P---> 3D	1.31E+04	1.31E+04	0.06766	0.00808	0.00810	0.22299	6.83673	6.85200	0.22289
3P---> 3D	7.87E+04	7.87E+04	0.03967	0.07279	0.07294	0.20465	61.53188	61.66000	0.20778
3P---> 4S	6.43E+07	6.47E+07	0.52107	0.13379	0.13470	0.67532	9.28874	9.35400	0.69765
3P---> 4D	1.88E+07	1.82E+07	3.32882	0.05356	0.05210	2.79398	3.07645	2.99000	2.89129
3P---> 4D	1.13E+08	1.09E+08	3.51579	0.48198	0.46800	2.98689	27.68647	26.90000	2.92369
3P---> 5S	2.75E+07	2.77E+07	0.82634	0.02162	0.02190	1.29939	0.92302	0.93400	1.17561
3P---> 5D	9.62E+06	9.32E+06	3.22688	0.01337	0.01300	2.86369	0.53665	0.52100	3.00402
3P---> 5D	5.77E+07	5.60E+07	3.07923	0.12035	0.11700	2.86275	4.82980	4.69000	2.98074
3P ---> 6S	1.46E+07	1.47E+07	0.39090	0.00798	0.00805	0.89821	0.28347	0.28600	0.88372
3P---> 6D	5.45E+06	5.30E+06	2.85441	0.00560	0.00545	2.66536	0.19296	0.18800	2.63879
3P---> 6D	3.27E+07	3.18E+07	2.85441	0.05036	0.04900	2.77012	1.73665	1.69000	2.76026
3P---> 7S	8.78E+06	8.89E+06	1.19304	0.00396	0.00402	1.40251	0.12817	0.13000	1.40543
3P---> 7D	2.03E+07	1.97E+07	2.86863	0.02651	0.02580	2.76381	0.84286	0.82100	2.66316
3P---> 7D	3.38E+06	3.29E+06	2.66163	0.00295	0.00287	2.64566	0.09365	0.09130	2.57678
3P---> 8D	1.34E+07	1.30E+07	3.23238	0.01590	0.01550	2.60159	0.48116	0.46800	2.81244
3P---> 8D	2.24E+06	2.17E+06	3.07720	0.00177	0.00172	2.73724	0.05346	0.05200	2.81540
3D---> 4P	8.42E+06	8.76E+06	3.88555	0.01469	0.01530	3.95545	0.93455	0.97400	4.05022
3D---> 4P	8.42E+05	8.77E+05	4.03629	0.00294	0.00307	4.31682	0.18681	0.19500	4.20095
3D---> 4F	2.07E+08	2.07E+08	0.14122	1.01686	1.02000	0.30771	62.59556	62.50000	0.15289
3D---> 5P	3.55E+06	3.74E+06	5.21302	0.00278	0.00293	5.28647	0.11820	0.12500	5.44109
3D---> 5P	3.54E+05	3.74E+05	5.25275	0.00055	0.00059	5.49007	0.02363	0.02500	5.48466
3D---> 5F	6.85E+07	6.82E+07	0.36725	0.15715	0.15700	0.09618	6.61805	6.61000	0.12179
3D---> 6F	3.24E+07	3.22E+07	0.53169	0.05414	0.05400	0.26629	1.94619	1.94000	0.31928
3D---> 7F	1.82E+07	1.81E+07	0.64236	0.02572	0.02570	0.09470	0.84963	0.84800	0.19206
3D---> 8F	1.14E+07	1.14E+07	0.16914	0.01450	0.01450	0.02436	0.45506	0.45500	0.01312
3D---> 9F	7.63E+06	7.29E+06	4.66193	0.00909	0.00870	4.47384	0.27572	0.26400	4.44091
3D---> 4P	7.58E+06	7.87E+06	3.74730	0.01763	0.01830	3.67591	1.68155	1.75000	3.91134
3D---> 4F	1.48E+07	1.47E+07	0.72076	0.04842	0.04830	0.25314	4.47125	4.46000	0.25223
3D---> 4F	2.22E+08	2.21E+08	0.49412	0.96845	0.96600	0.25315	89.42446	89.20000	0.25163
3D---> 5P	3.19E+06	3.37E+06	5.35752	0.00333	0.00352	5.42545	0.21269	0.22500	5.47212
3D---> 5F	4.89E+06	4.87E+06	0.38989	0.00748	0.00747	0.17574	0.47271	0.47200	0.15040
3D---> 5F	7.33E+07	7.31E+07	0.32401	0.14967	0.14900	0.44701	9.45440	9.44000	0.15251

Transition	Transition Probability (s^{-1})			Oscillator Strength			Line Strength (a.u.)		
	This work	NIST	% Error	This work	NIST	% Error	This work	NIST	% Error
3D---> 6F	2.31E+06	2.31E+06	0.08872	0.00258	0.00258	0.07168	0.13901	0.13900	0.00656
3D---> 6F	3.47E+07	3.46E+07	0.23588	0.05156	0.05160	0.06933	2.78025	2.78000	0.00882
3D---> 7F	1.30E+06	1.30E+06	0.08110	0.00122	0.00122	0.40162	0.06069	0.06060	0.14053
3D---> 7F	1.95E+07	1.94E+07	0.59698	0.02450	0.02440	0.40162	1.21370	1.21000	0.30606
3D---> 8F	1.22E+07	1.22E+07	0.06407	0.01381	0.01380	0.08415	0.65003	0.64900	0.15927
3D---> 8F	8.13E+05	8.11E+05	0.22672	0.00069	0.00069	0.05751	0.03250	0.03250	0.00833
3D---> 9F	8.17E+06	7.81E+06	4.65556	0.00866	0.00828	4.53266	0.39385	0.37700	4.46854
3D---> 9F	5.45E+05	5.19E+05	4.99841	0.00043	0.00041	4.79243	0.01969	0.01880	4.75300
4S---> 4P	2.77E+06	2.75E+06	0.66270	0.38134	0.37900	0.61676	76.17664	75.80000	0.49689
4S---> 4P	2.77E+06	2.76E+06	0.37181	0.76286	0.76100	0.24461	152.35308	152.00000	0.23229
4S---> 5P	2.60E+06	2.55E+06	1.98133	0.02133	0.02090	2.06587	1.03984	1.02000	1.94543
4S---> 5P	2.60E+06	2.53E+06	2.70066	0.04262	0.04160	2.46339	2.07773	2.03000	2.35129
4P---> 4D	2.13E+04	2.12E+04	0.24055	0.14572	0.14500	0.49592	145.22058	145.00000	0.15212
4P---> 5S	1.01E+07	1.02E+07	0.97198	0.20560	0.20700	0.67529	15.78776	15.90000	0.70592
4P---> 5D	1.86E+07	1.81E+07	2.54131	0.49915	0.48700	2.49480	31.15305	30.40000	2.47715
4P---> 6S	4.87E+06	4.89E+06	0.40074	0.03329	0.03350	0.61285	1.48162	1.49000	0.56210
4P---> 6D	1.15E+07	1.11E+07	3.25888	0.13535	0.13200	2.53671	5.59755	5.45000	2.70733
4P---> 7S	2.82E+06	2.84E+06	0.73776	0.01238	0.01250	0.93892	0.44170	0.44500	0.74178
4P---> 7D	7.28E+06	7.05E+06	3.21387	0.05934	0.05760	3.01335	2.03917	1.98000	2.98841
4P---> 8D	4.87E+06	4.73E+06	2.96452	0.03225	0.03140	2.70910	0.99880	0.97200	2.75676
4P---> 4D	4.23E+03	4.22E+03	0.34487	0.01455	0.01450	0.37193	29.04389	29.00000	0.15134
4P---> 4D	2.54E+04	2.54E+04	0.13973	0.13104	0.13100	0.02692	261.39950	261.00000	0.15307
4P---> 5S	2.02E+07	2.03E+07	0.47998	0.20565	0.20700	0.65235	31.58579	31.80000	0.67361
4P---> 5D	3.71E+06	3.62E+06	2.55197	0.04993	0.04880	2.31112	6.23269	6.09000	2.34309
4P---> 5D	2.23E+07	2.17E+07	2.64190	0.44932	0.43900	2.35082	56.08982	54.80000	2.35370
4P---> 6S	9.74E+06	9.81E+06	0.70469	0.03330	0.03360	0.89717	2.96375	2.99000	0.87776
4P---> 6D	2.29E+06	2.23E+06	2.79870	0.01354	0.01320	2.55000	1.11971	1.09000	2.72586
4P---> 6D	1.38E+07	1.34E+07	2.64526	0.12183	0.11900	2.37764	10.07741	9.82000	2.62125
4P---> 7S	5.64E+06	5.68E+06	0.73799	0.01238	0.01250	0.93046	0.88351	0.89100	0.84035
4P---> 7D	8.73E+06	8.48E+06	2.97136	0.05341	0.05190	2.90440	3.67103	3.57000	2.83006
4P---> 7D	1.46E+06	1.41E+06	3.21356	0.00593	0.00578	2.66527	0.40788	0.39700	2.74171
4P---> 8D	5.84E+06	5.68E+06	2.89109	0.02903	0.02830	2.57142	1.79804	1.75000	2.74497

Transition Probabilities, Oscillator Strengths and Line Strengths Result From Radiative Transitions

Transition	Transition Probability (s^{-1})			Oscillator Strength			Line Strength (a.u.)		
	This work	NIST	% Error	This work	NIST	% Error	This work	NIST	% Error
4P---> 8D	9.74E+05	9.44E+05	3.18063	0.00323	0.00313	3.04307	0.19978	0.19400	2.97837
4D---> 5P	4.40E+06	4.52E+06	2.55204	0.03614	0.03710	2.59979	4.98251	5.12000	2.68533
4D---> 5P	4.40E+05	4.50E+05	2.15896	0.00722	0.00740	2.38527	0.99596	1.02000	2.35684
4D---> 5P	3.96E+06	4.06E+06	2.39098	0.04335	0.04450	2.59078	8.96514	9.21000	2.65861
5S---> 5P	8.58E+05	8.52E+05	0.69750	0.47943	0.47700	0.51015	192.89522	192.00000	0.46626
5S ---> 5P	8.59E+05	8.53E+05	0.65754	0.95911	0.95500	0.43008	385.78580	384.00000	0.46505
5P---> 5D	7.80E+03	7.82E+03	0.31887	0.20361	0.20500	0.67567	396.04773	398.00000	0.49052
5P---> 6S	3.91E+06	3.93E+06	0.51046	0.27837	0.28100	0.93517	39.97715	40.30000	0.80111
5P---> 6D	5.37E+06	5.27E+06	1.96922	0.49341	0.48500	1.73420	56.90054	55.90000	1.78987
5P ---> 7S	2.04E+06	2.06E+06	0.73352	0.04499	0.04530	0.67437	3.59222	3.62000	0.76749
5P---> 7D	3.69E+06	3.61E+06	2.35056	0.13814	0.13500	2.32383	10.16507	9.95000	2.16148
5P---> 8D	2.53E+06	2.47E+06	2.27064	0.06193	0.06060	2.20119	3.69073	3.61000	2.23623
5P---> 5D	1.55E+03	1.56E+03	0.44404	0.02034	0.02040	0.31598	79.20922	79.60000	0.49092
5P---> 5D	9.33E+03	9.35E+03	0.23009	0.18309	0.18400	0.49608	712.89235	716.00000	0.43403
5P---> 6S	7.82E+06	7.87E+06	0.63188	0.27844	0.28100	0.91161	79.98082	80.60000	0.76821
5P---> 6D	1.07E+06	1.06E+06	1.40900	0.04936	0.04860	1.55716	11.38458	11.20000	1.64807
5P---> 6D	6.45E+06	6.35E+06	1.56870	0.44421	0.43800	1.41804	102.46126	101.00000	1.44679
5P---> 7S	4.09E+06	4.12E+06	0.73250	0.04500	0.04540	0.88180	7.18563	7.25000	0.88785
5P---> 7D	4.43E+06	4.33E+06	2.41051	0.12435	0.12200	1.92798	18.30232	17.90000	2.24760
5P---> 7D	7.39E+05	7.22E+05	2.35938	0.01382	0.01350	2.34248	2.03348	1.99000	2.18501
5P---> 8D	3.03E+06	2.96E+06	2.41923	0.05575	0.05450	2.29566	6.64487	6.50000	2.22876
5P---> 8D	5.05E+05	4.93E+05	2.48346	0.00619	0.00606	2.21451	0.73827	0.72200	2.25354

Conclusion

An extensive study has been carried out by employing the single-electron approximation and quantum defect theory to calculate transition probabilities, oscillator strengths, and line strength of 6386 transitions of ionic states of beryllium ion. The salient findings of this research work are appended below.

1. The transition probabilities are compared with NIST data. While there are isolated cases with an error margin of 5%, the majority exhibit errors of less than 1%.
2. The 6386 transitions have been presented in the supplementary table. This table contains transition wavelength, energies, transition probabilities, oscillator strengths, line strengths, configurations, and terms of upper and lower levels. Out of 6386 transitions, only 149 are listed in the NIST database. Table 2 shows both calculated values and NIST values for 149 transitions.
3. The transition probabilities have been used to calculate the lifetimes of nS, nP, nD, and nF states. The lifetimes of 112 states are reported in this article for principal quantum number $n < 31$. Most of the lifetimes are presented for the first time. The lifetimes are also compared with the available published data.
4. The lifetimes are compared with the corresponding works of [3-9, 18, 19, 21-31].

The lifetimes for both sets computed in this work show excellent agreement with the results of CAHS [21], FMP [18], WBEPMT, QDOT [19], RMBT [29], and [30, 31].

5. The lifetimes of nS, nP, nD, and nF states exhibit a monotonically increasing trend, with an exception observed at the 3P state, where the lifetime is lesser than that of the 2P state.
6. A Python program was developed to calculate the radial integral. The same program was used to calculate the corresponding expectation values $\langle r \rangle$ to check the validity of the results.

Compliance with Ethical Standards

The authors certify that they have complied with the Journal's ethical guidelines.

Funding:

There is no funding for this work.

Conflict of Interest:

There is no conflict of interest.

Ethical Conduct

The authors are well aware of their ethical responsibilities.

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