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MEAN LIFETIMES OF ns, np, nd, & nf LEVELS OF N V[†]

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Nitrogen is one of the key elements in the evolution and formation of stellar objects. Earth's atmosphere contains 21% oxygen and 78% nitrogen; these two gases give rise to aurora when ions of the solar wind in the ionosphere collide with them. Some aerosols made of nitrogen and oxygen are also found in the atmosphere. Nitrogen, hydrogen, carbon, and oxygen are the main contributors to the origin of life on Earth. The spectrum of nitrogen ion (N V) has been studied using Quantum defect theory (QDT) and Numerical Coulombic approximation (NCA). N V has two electrons in the core, with the nucleus, and one electron outside the core. It makes it hydrogen or lithium-like. In the first part, the energies of the ns, np, nd, and nf up to n < 30 were calculated with the help of QDT. In the second part, the wavelengths were calculated using the energies and line strength parameters using NCA. Very little experimental data on lifetime and transition probability are available; however, Biemont et al. have calculated the lifetime of the 48 levels of N V using coulomb approximation. In this study, we calculated the lifetime of 196 multiplets of N V. The results are compared with the available experimental and theoretical lifetimes; an excellent agreement was found between known lifetimes and calculated in this work. The lifetimes of 100 multiplets are presented for the first time. The lifetimes of each of the Rydberg series of N V were fitted, and a third-degree polynomial represents the lifetimes of each series.
Keywords: *Nitrogen ion (N V); Lifetimes; Quantum defect theory; Numerical coulomb approximation; Lithium-like ions*
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INTRODUCTION

In the evolution of chemically peculiar stars, nitrogen plays an important role. For example, Pluto is believed to have a rocky core and layers of various ices in the surface crust; most of the ice is nitrogen. It indicates a high abundance of nitrogen on Pluto. Improved spectroscopic data is essential in determining reliable values of stellar abundances. Kancerecivius calculated transition probabilities and Oscillator Strengths using analytic wave functions of helium and lithium-like atoms from np to ms (m<3, n <6). They used three different expressions for the dipole moments [1]. Fischer et al. calculated transition data, including lifetimes using the multiconfiguration Breit-Pauli method of the Li sequence. They calculated the lifetimes of all configuration levels of principal quantum number < 4, including the configuration $1s^2 4s$ [2]. Mohammed El-Mekki used a semi-empirical Couloum Approximation to calculate 2p levels of isoelectronic Li-sequence lifetimes. With the help of Hartree Slater's core, he calculated lifetimes for Z =3 – 92 [3]. Chen and Crasemann used the Multiconfiguration Dirac-Fock approach to calculate the transition data of the highest spin metastable $^4F_{9/2}$ of 1s 2p 3d configuration of Li-like ions for Z = 6 to 42. They calculated Auger energies, Auger rate, radiative energies, and radiative rate for the transition 2s - 2p, 3p – 3d, 1s – 2p, and 2s-3d [4]. Blanke et al. studied decay curves of the quartet system of Li-like ions for n = 6 – 9. The decay curve measured the lifetimes of n = 3 states of the configuration 1s 2p 3d [5]. Tunnell and Bhalla estimated the lifetimes of the ^4P state of the configuration $1s\,2p^2$ of the lithium-like ions (Z = 7, 8, 10, and 12) [6]. Kernahan et al. measured the lifetimes of 11 levels belonging to N II – N V. They considered the transition below 500Å [7]. Baudinet-Robinet and P. D. Dumont used the beam foil technique to measure the lifetimes of N V levels in the ultraviolet spectrum range. Using Coulomb approximation, they found branching fractions and combined them with the lifetime to measure the transition probabilities [8]. Kernahan et al. also used the beam-foil technique to measure the lifetimes of 41 states of N I – N V. They studied transitions in the range 374 to 2064Å. They compared the results with existing known lifetimes and found that they agree well for levels near the ionization stage [9]. Dumont also used the beam-foil technique to measure the lifetime of nitrogen in the UV spectrum range. They studied nitrogen spectra and found lifetimes of 24 levels in the range 650 – 2000Å [10]. Desesquelles used the technique of beam of ions by a thin Carbon foil to prepare a nitrogen beam. This technique can make an ions beam between 100 keV and 16 MeV. Most of the lines of the spectra of neutral nitrogen to N VII can be observed. The lifetimes of upper levels and transition probabilities were found by the spatial decay of the light emitted by fast-moving atoms and ions [11]. Lewis et al. also used the foil excitation technique at high energy of 2 MeV of nitrogen through carbon foil and measured the lifetimes of upper levels of the transition in N II to N V. The transition lines they observed were in the range of 2000 to 5000Å. The measured lifetime by the spatial decay of the excited levels was 0.4 to 10 ns [12]. Heroux also used the same technique Desesquelles [10] and Lewis [12] used to measure the lifetime of multiplets in N II to N V. The beam energy of nitrogen ions was the same as used by Lewis [12], but the range of wavelengths was from 1085 to 162Å [13]. Berry et al. studied nitrogen transition in N I-VI using the beam foil technique; they used an energy range of 0.25-2.0 MeV in wavelength range 1050-3000Å and 5.5 Mev between 2000-5000Å [14].

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THEORY

Quantum mechanical systems are complex systems; the exact analytical solutions of the systems are often unavailable or impossible to find. Numerical approaches are one of the best alternatives to reach an approximate solution. Schrödinger equation can be solved analytically for hydrogen atoms, with the approximation that variables are separable, but this equation is difficult to solve for helium and other elements. If the system is approximated as hydrogen, the solution is achievable and close to the exact solution in many cases, such as Li and lithium-like ions. Nitrogen ion (N V) is a lithium-like ion; its transition data can be obtained by numerically solving the Schrödinger equation.

$$\left(\frac{d^2}{dr^2} - 2V(r) - \frac{l^*(l^*+1)}{r^2} + 2E\right)P(r) = o. \tag{1}$$

The equation (1) can be written as

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

Here $R(r) = \frac{P(r)}{r}$, $A/r_i - B/r_i^2 = V(r_i)$ is the potential observed by the electron outside the core formed by the nucleus and other electrons in the atom, $A = -z^*$ is the effective nuclear charge where r_i is the distance between electron i and the nucleus.

The solution of equation (2) gives the radial wavefunction R as:

$$R = Cexp\left(-\frac{Z^*r}{n^*}\right) r^{l^*} L_{n^*-l^*-1}^{2l^*+1}\left(\frac{2Z^*r}{n^*}\right). \tag{3}$$

Where $C = \left(\frac{2Z^*}{n^*}\right)^{l^*+\frac{3}{2}} \sqrt{\frac{(n^*-l^*-1)!}{2n^*\Gamma(n^*+l^*+1)}}$, n^* is the effective principal quantum number. The lifetime can be calculated using equation (4)

$$\tau_i = \left(\frac{\lambda(\text{Å})}{1265.38}\right)^3 \frac{g_i}{S_{if}}, \tag{4}$$

where the line strength factor S_{if} is given by,

$$S_{if} = \sum_{n_i,n_f} [< f|r|i >]^2. \tag{5}$$

The matrix element values in equation (5) can be obtained using the wavefunctions in equation (3).

RESULT AND DISCUSSION

Quantum defect theory (QDT) and Numerical Coulombic approximation (NCA) were used to study the lifetimes of the nitrogen ion (N V). The energies and quantum defects were calculated with the help of QDT. These energies and quantum defects were used to calculate the lifetimes of the levels of N V. The lifetimes of any branch of the transition depend on the transition wavelength and line strength parameter. The wavelengths were calculated by the difference of energies of upper and lower levels calculated by QDT. The wavefunctions of upper and lower levels are required to calculate line strength parameters. Since nitrogen ion (N V) may be considered hydrogen-like, hydrogen wavefunction can be used to calculate the matrix element needed for the line strength parameters. The matrix elements are calculated using NCA.

The lifetimes of the Rydberg Series $1s^2$ ns, $1s^2$ np, $1s^2$ nd, and $1s^2$ nf levels of N V have been calculated and compared with the available experimental and theoretical values. Generally, a good agreement is found between calculated and available lifetime data. It was found that the available experimental data on lifetime is very little. The most detailed theoretical work on the lifetime of N V is by Biemont et al. However, they reported lifetimes of forty-eight levels of N V. In this work, the lifetimes of 196 multiplets are presented. Table 1 gives the lifetimes of N V levels; the first column gives the configuration, the second column gives the angular momentum third columns give the lifetimes calculated in this work, and the fourth and last column gives the corresponding lifetimes available in the literature. The lifetime calculated for $1s^2$ 2p is slightly different from the experimental value. The reason could be its closeness to the core, which may affect the effective charge compared to the other levels that lie relatively far from the core. It was observed in the calculations of transition probability and lifetimes of the same configuration in Li I [16], Be II [17], and C IV [18] that the calculated and experimental values are slightly different. For the configuration $1s^2$ 2p in Li-like atoms and ions, one should expect a slight difference in theoretical and experimental lifetimes. A study is needed to see if the problem is resolved by changing Z by its effective value.

Table 1. The lifetimes of multiplets of N V calculated in this work and compared with available data

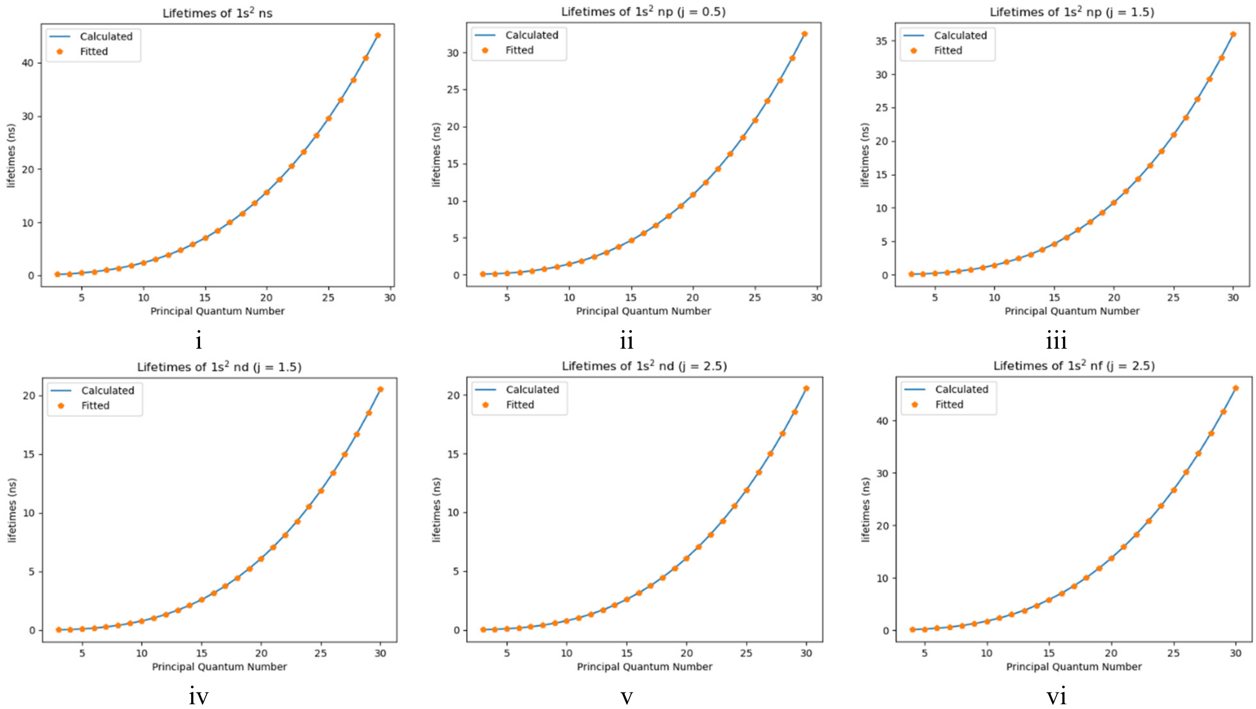
Term $1s^2.nl$	J	This work	Other works
3d	3/2	0.0228	0.02[g]
3d	5/2	0.0228	
4d	3/2	0.0527	0.065[a], 0.05[g]
4d	5/2	0.0527	0.95[d]
5d	3/2	0.1012	0.1[g]
5d	5/2	0.1012	
6d	3/2	0.1726	0.18[g]
6d	5/2	0.1728	
7d	3/2	0.2715	0.28[g]
7d	5/2	0.2718	
8d	3/2	0.4024	0.41[g]
8d	5/2	0.4028	
9d	3/2	0.5698	0.59[g]
9d	5/2	0.5703	
10d	3/2	0.7781	0.8[g]
10d	5/2	0.7789	
11d	3/2	1.032	1.05[g]
11d	5/2	1.033	
12d	3/2	1.3359	1.37[g]
12d	5/2	1.3372	
13d	3/2	1.6943	1.77[g]
13d	5/2	1.6959	
14d	3/2	2.1118	2.12[g]
14d	5/2	2.1139	
15d	3/2	2.5929	2.53[g]
15d	5/2	2.5955	
16d	3/2	3.1421	3.19[g]
16d	5/2	3.1453	
17d	3/2	3.7639	3.73[g]
17d	5/2	3.7678	
18d	3/2	4.463	4.75[g]
18d	5/2	4.4675	
19d	3/2	5.2437	
19d	5/2	5.2491	
20d	3/2	6.1106	
20d	5/2	6.117	
21d	3/2	7.0684	
21d	5/2	7.0758	
22d	3/2	8.1214	
22d	5/2	8.1299	
23d	3/2	9.2742	
23d	5/2	9.284	
24d	3/2	10.5314	
24d	5/2	10.5425	
25d	3/2	11.8974	
25d	5/2	11.91	
26d	3/2	13.3769	
26d	5/2	13.3911	
27d	3/2	14.9743	
27d	5/2	14.9903	
28d	3/2	16.6942	
28d	5/2	16.7118	
29d	3/2	18.541	
29d	5/2	18.5608	
30d	3/2	20.5184	
30d	5/2	20.538	
10f	5/2	1.7395	
11f	5/2	2.3098	
12f	5/2	2.9928	
13f	5/2	3.7989	
14f	5/2	4.738	
15f	5/2	5.8205	
16f	5/2	7.0566	
17f	5/2	8.4564	
18f	5/2	10.0302	
19f	5/2	11.7882	
20f	5/2	13.7405	
21f	5/2	15.8974	
22f	5/2	18.2692	
23f	5/2	20.8659	
24f	5/2	23.6978	
25f	5/2	26.7752	
26f	5/2	30.1082	
27f	5/2	33.7071	
28f	5/2	37.5821	
29f	5/2	41.7421	
30f	5/2	46.1474	
4f	5/2	0.1153	0.12[g]
4f	7/2	0.1153	
5f	5/2	0.223	0.22[g]
5f	7/2	0.2231	
6f	5/2	0.3823	0.61[d], 0.38[g]
6f	7/2	0.3824	
7f	5/2	0.6034	0.6[g]
7f	7/2	0.6036	
8f	5/2	0.8965	0.89[g]
8f	7/2	0.8968	
9f	5/2	1.2718	1.26[g]
9f	7/2	1.2723	
10f	7/2	1.7402	1.72[g]
11f	7/2	2.3107	
12f	7/2	2.994	
13f	7/2	3.8004	
14f	7/2	4.7399	
15f	7/2	5.8229	
16f	7/2	7.0596	
17f	7/2	8.46	
18f	7/2	10.0345	
19f	7/2	11.7932	
20f	7/2	13.7465	
21f	7/2	15.9044	
22f	7/2	18.2771	
23f	7/2	20.8751	
24f	7/2	23.7083	

Term 1s^2.nl	J	This work	Other works
25f	7/2	26.787	
26f	7/2	30.1216	
27f	7/2	33.7221	
28f	7/2	37.5987	
29f	7/2	41.762	
30f	7/2	46.2199	
2p	3/2	2.8423	2.9741[a] , 3.12[b] , 3.2[d] , 3.3[f] , 2.95[g]
2p	1/2	2.871	2.9442[a], 3.08[b], 3.3[d], 3.3[f]
3p	1/2	0.0821	0.081328[a] , 0.084[e] , 0.51[f] 0.08[g]
3p	3/2	0.0822	0.082058[a]
4p	1/2	0.1333	0.14[g], 0.17[e]
4p	3/2	0.1335	
5p	1/2	0.2224	0.22[g]
5p	3/2	0.2227	
6p	1/2	0.353	0.51[f], 0.36[g]
6p	3/2	0.3534	
7p	1/2	0.5321	0.54[g]
7p	3/2	0.5327	
8p	1/2	0.7672	0.77[g]
8p	3/2	0.7679	
9p	1/2	1.0659	1.08[g]
9p	3/2	1.0669	
10p	1/2	1.436	1.46[g]
10p	3/2	1.4373	
11p	1/2	1.8854	1.85[g]
11p	3/2	1.887	
12p	1/2	2.4219	2.45[g]
12p	3/2	2.4239	
13p	1/2	3.0532	2.96[g]
13p	3/2	3.0557	
14p	1/2	3.7873	3.92[g]
14p	3/2	3.7904	
15p	1/2	4.632	4.26[g]
15p	3/2	4.6357	
16p	1/2	5.5951	4.3[g]
16p	3/2	5.5996	
17p	1/2	6.6846	5.03[g]
17p	3/2	6.6899	
18p	1/2	7.9083	
18p	3/2	7.9145	
19p	1/2	9.2741	
19p	3/2	9.2814	
20p	1/2	10.7899	
20p	3/2	10.7983	
21p	1/2	12.4635	
21p	3/2	12.4731	

Term 1s^2.nl	J	This work	Other works
22p	1/2	14.3028	
22p	3/2	14.3138	
23p	1/2	16.3157	
23p	3/2	16.3282	
24p	1/2	18.5101	
24p	3/2	18.5242	
25p	1/2	20.8939	
25p	3/2	20.9098	
26p	1/2	23.4749	
26p	3/2	23.4927	
27p	1/2	26.2611	
27p	3/2	26.2809	
28p	1/2	29.26	
28p	3/2	29.2821	
29p	1/2	32.4742	
29p	3/2	32.5049	
30p	1/2	35.906	
30p	3/2	35.9494	
3s	1/2	0.11	0.10985[a] , 0.121[c] , 0.12[e] , 0.11[g]
4s	1/2	0.1733	0.5[a] , 0.17212[e] , 0.18[g]
5s	1/2	0.2849	0.29[g]
6s	1/2	0.4486	0.45[g]
7s	1/2	0.6731	0.68[g]
8s	1/2	0.9678	0.98[g]
9s	1/2	1.3425	1.39[g]
10s	1/2	1.8069	1.84[g]
11s	1/2	2.3709	
12s	1/2	3.0444	
13s	1/2	3.8375	
14s	1/2	4.7599	
15s	1/2	5.8216	
16s	1/2	7.0327	
17s	1/2	8.403	
18s	1/2	9.9426	
19s	1/2	11.6614	
20s	1/2	13.5694	
21s	1/2	15.6766	
22s	1/2	17.993	
23s	1/2	20.5286	
24s	1/2	23.2933	
25s	1/2	26.2971	
26s	1/2	29.5501	
27s	1/2	33.0623	
28s	1/2	36.843	
29s	1/2	40.8972	
30s	1/2	45.1651	

[a][2], [b][7], [c][9], [d][10], [e][13], [f][14], [g][15]

The plot of lifetimes is smoothly increasing; the different polynomials were fitted on the calculated lifetime's data of N V. Third-degree polynomial ($\tau = a_o + a_1 n + a_2 n^2 + a_3 n^3$) fitting gives closer values of calculated lifetimes. Figure 1(i)-1(vii) gives plots of calculated lifetimes with fitted values for 1s^2 ns, 1s^2 np, 1s^2 nd, and 1s^2 nf levels of N V. In fitting the np series, the level 1s^2 2p was not included as its lifetime does not follow the trend.



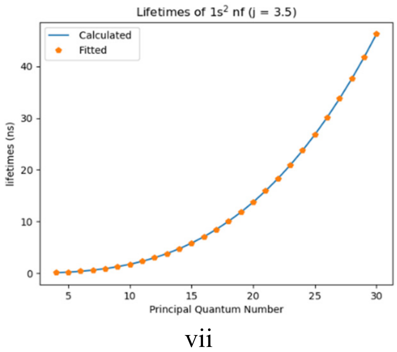


Figure 1. The plot of lifetimes calculated in this work with the fitted values for (i) ns (j = 0.5), (ii) np (j = 0.5), (iii) np (j = 1.5), (iv) nd (j = 1.5), (v) nd (j = 2.5), (vi) nf (j = 2.5), (vii) ng (j = 3.5) levels of N V

Third-degree polynomial represents the lifetimes of various Rydberg series $1s^2$ ns, $1s^2$ np, $1s^2$ nd, $1s^2$ nf of N V. The coefficients of the polynomials are given in Table 2. There are two polynomials for each of the series np, nd, and nf for two different possible values of angular momentum. nd series is the only series for which the coefficients for both angular momenta are approximately the same.

Table 1. Coefficients of the polynomial fitted for calculated lifetimes of N V for different series

	Coefficients of the Polynomial			
Term and J value	a_o	a_1	a_2	a_3
ns (1/2)	0.053562	0.009137	0.005815	0.00164
np (1/2)	0.019362	0.005954	0.000504	0.001306
np (3/2)	0.017367	0.006626	0.000449	0.001309
nd (3/2)	-0.0035	0.001466	0.000128	0.000754
nd (5/2)	-0.0034	0.001432	0.00013	0.000755
nf (5/2)	0.018192	-0.00479	0.000773	0.001689
nf (7/2)	-0.00463	0.001625	0.000275	0.001701

CONCLUSIONS

The Rydberg levels series $1s^2$ ns, $1s^2$ np, $1s^2$ nd, and $1s^2$ nf of N V have been studied. The lifetimes of multiplets belonging to these levels have been calculated and compared with the available data. The agreement is excellent except for $1s^2$ 2p levels, where a slight difference between calculated and experimental values of lifetimes was observed. The same can be observed in all Lithium like ions due to the cooper minimum. The cooper minimum was first observed for alkali atoms. It occurs due to overlapping the positive and negative amplitude of the wavefunctions of the levels taking part in the transition [16]. Due to this, the dipole matrix elements have zero or a minimum value for a particular set of principal quantum numbers of both levels. According to Fano and Cooper [19], the oscillator strength as a function of effective principal quantum number (n*) drops rapidly towards a minimum, where a reversal sign in the R integral occurs. QDT and NCA were used to calculate energy, quantum defects, and lifetimes of N V. The lifetimes of 196 multiplets were calculated, but the available experimental data was insufficient. However, Biemont et al. theoretically determined the lifetimes of forty-eight levels; hence, 100 lifetimes presented in this paper are new. The plot of lifetimes against the principal quantum number follows a polynomial, so different polynomials were fitted, and in each series third-degree polynomial fits well on the calculated lifetimes of the N V Rydberg series.

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СЕРЕДНІЙ ЧАС ЖИТТЯ РІВНІВ ns, np, nd та nf у N V

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Азот є одним із ключових елементів еволюції та формування зоряних об’єктів. Атмосфера Землі містить 21% кисню і 78% азоту; ці два гази викликають полярне сяйво, коли з ними стикаються іони сонячного вітру в іоносфері. Деякі аерозолі з азоту та кисню також знаходяться в атмосфері. Азот, водень, вуглець і кисень є головними причинами виникнення життя на Землі. Спектр іонів азоту (N V) досліджено за допомогою квантової теорії дефектів (КТД) і чисельного кулонівського наближення (НКА). N V має два електрони в ядрі з ядром і один електрон поза ядром. Це робить його подібним до водню або літію. У першій частині за допомогою QDT розраховано енергії ns, np, nd та nf до n < 30. У другій частині довжини хвиль були розраховані з використанням параметрів енергії та сили лінії за допомогою NCA. Доступно дуже мало експериментальних даних щодо тривалості життя та ймовірності переходу; однак Biemont et al. розрахували час життя 48 рівнів N V, використовуючи кулонівське наближення. У цьому дослідженні ми розрахували тривалість життя 196 мультиплетів N V. Результати порівнюються з доступними експериментальними та теоретичними тривалістю життя; У цій роботі було знайдено відмінну відповідність між відомими і розрахованими часами життя. Тривалість життя 100 мультиплетів представлена вперше. Часи життя кожного ряду Рідберга N V були підібрані поліномом третього ступеня яким представлено час життя кожного ряду.
Ключові слова: *іон азоту (N V); терміни життя; квантова теорія дефектів; числова кулонівська апроксимація; літієподібні іони*