

Resonance Parameters, Autoionisation of $^{2S+1}L^o$ Doubly Excited N^{5+} Ion States Associated with $n=3$ and 4, N^{6+} Threshold

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Abstract: The motivation of the diagonalization method is to take into consideration the coupling between closed and opened channels in term of perturbation theory and to neglect the indirect coupling as well but also the autoionisation states through the opened channels. This procedure leads to a relatively simple mathematical problem consisting of solving a system of linear algebraic equations instead of a system of coupled differential equations or integro-differential equations. Diagonalization method under LS coupling scheme for the states $^{1,3}P^o$, $^{1,3}D^o$, $^{1,3}F^o$, $^{1,3}G^o$, $^{1,3}H^o$ was performed. The partial widths for multi-channel autoionizing levels to sublevels of N^{6+} were carried out by neglecting the direct coupling between opened channels. The calculations of total and partial widths of the $(nln'l')^{1,3}L^o$ ($L=1, 2, 3, 4$ and 5) multiple-decay-channel system N^{5+} were performed. From $L=1$ to 2, the $(4l4l')^{1,3}L^o$ states located under $n=3$ and the $(3lnl')^{1,3}L^o$ states follow the same rules. All the $(4l4l')^{1,3}G^o$ and $(4l4l')^{1,3}H^o$ states located under $n=3$ observe the rule 1.

Keywords: Autoionisation, Electron Correlation, Partial Width

1. Introduction

Recently, there has been considerable interest in experimental investigations [1-6] and theoretical studies of resonant photoionization of helium-like ions and properties of autoionizing states has been renewed by the advent of high-energy resolution spectrometers using synchrotron radiation and the appearance of multiply charged ions sources like electron cyclotron resonance or electron-beam ion source. Doubly excited states in He-like ions have been intensively studied in connection with the understanding of collisional and radiational processes which take place in hot astrophysical and laboratory plasmas.

Considerable interest is remaining in experimental investigations of electron-transfer collisions between a highly stripped ion and a two-electron helium atom. In such processes,

although one-electron captures would dominate the electron-transfer collisions, it was found that two-electron capture processes are also important. For example, the production of doubly excited autoionisation states of N^{5+} ions [2] below the $n=3$ and $n=4$ thresholds in collisions of N^{6+} ions with He atoms. To interpret and identify satellite lines of such highly stripped ions, which in turn would play an important role in spectroscopic diagnostics of high-temperature astrophysical and laboratory plasmas, knowledge of the doubly excited autoionizing states are needed.

From the theoretical side, a set of calculation of the characteristics of double excited resonances in helium-like ion is still going on [7] and have been carry out by various methods using different approaches. Based on the literature [8-12, 14] several approaches were developed as well as the computing double-sum over the complete hydrogen spectrum

[15], the density functional theory [16], the Feshbach-projection formalism [17], and the spin-dependent localized Hartree-Fock density-functional method [18], the method combining Hylleraas and incomplete hydrogenic wave functions [19] and semi-empirical method [20]. For most of the preceding methods, calculations are performed mainly for resonance energies and total widths.

The approximation method of diagonalization (see Ref. 29 and references there in) is used for the present investigation. Bound-state-type and no asymptotic wave functions are an asset and show advantage of this method throughout resonance parameters (both resonance positions, total and partial widths) are necessarily used. Such an advantage becomes apparent when we are calculating a resonance in which many channels are opened. In contrast with the region below the $n=2$ threshold where the autoionisation states decay via one opened channel, near the $n=3, 4$ threshold, the computation of the characteristics of autoionisation resonances is a multichannel problem associated with nine opened channels. Thus for solving this problem, one have to consider the interaction between an autoionisation level with several continua. The motivation of the diagonalization method is to take into consideration the coupling between closed and opened channels in term of perturbation theory and to neglect the indirect coupling as well but also the autoionisation states through the opened channels. This procedure leads to a relatively simple mathematical problem consisting of solving a system of linear algebraic equations instead of a system of coupled differential equations or integro-differential equations.

The diagonalization calculations of the excitation energies of the autoionisation states were carried out in the basis of configurations: $nln'l'$ with $n=3, 4$; $n' \geq 10$. The wave functions are described by ant symmetrized product of the hydrogenic wave functions.

The final state of N^{5+} , leaving the residual hydrogen-like ion N^{6+} in an excited state, is influenced by the asymptotic potential of the form $\sim r^{-2}$. With charge $(Z - 1)$ in the assessment of partial and total widths, the leaving electron is considered here to be free from the attractive Coulomb potential of the N^{6+} nucleus, and is described by the coulomb functions of the continuum spectrum.

The use of this method has been very successful for calculations of $L=1$ resonant states of two-electron atoms [21-24].

We now extend calculations to the partial autoionisation widths to 2ℓ and 3ℓ sublevels for resonance states $^{1,3}L^o$ with $L=1, 2, 3, 4$ and 5 quantum numbers. Our results are compared with the rare one obtained by the configuration-interaction method by Bachau and al [26], F Martin and al [32] and those obtained by Y. K. Ho [30] and Ho and Bathia [31] in the framework of complex-coordinate rotation method.

2. Theory

The final-state wave function is expanded based on the diagonalization approximation within the subspaces of closed

and opened channels as follows:

$$\psi_{Ei}(r_1, r_2) = \hat{A} \sum_k \psi_k(r_1) U_{ki}(E, r_2) + \sum_\mu \Lambda_\mu(E) \phi_\mu(r_1, r_2) \quad (1)$$

Where \hat{A} is the operator of anti symmetrization, k stands for a set of quantum numbers that characterize the ion + photoelectron system in the subspace of opened channels, $U_{ki}(E, r_2)$ is an unknown function which stands for the motion of the photoelectron.

$\psi_k(r_1)$ is the eigenfunction of residual ion satisfying the relations:

$$\langle \psi_k | \psi_{k'} \rangle = \delta_{kk'} \quad (2)$$

$$\langle \psi_k | \hat{H} | \psi_{k'} \rangle = \varepsilon_k \delta_{kk'} + V_{kk'} \quad (3)$$

The functions $\phi_\mu(r_1, r_2)$ was assess through unitary transformation of the Hamiltonian \hat{H} within the subspace of closed channels:

$$\phi_\mu(r_1, r_2) = \hat{A} \sum_{\ell m} \alpha_\mu [\psi_\ell(r_1) \psi_m(r_2)] \quad (4)$$

With the condition of diagonalization:

$$\langle \phi_\mu | \hat{H} | \phi_\nu \rangle = E_\mu \delta_{\mu\nu} \quad (5)$$

The coefficients α_μ of the unitary transformation (3) are found by solving the system of linear algebraic equations:

$$\sum_\nu \{ (E_\mu - E_0) \delta_{\mu\nu} - \langle \chi_\mu | \hat{V} | \chi_\nu \rangle \} = 0 \quad (6)$$

Where E_0 is the energy eigenvalue of the zero-order Hamiltonian corresponding to the \hat{H}_0 Eigen functions χ_μ defined by:

$$\chi_\mu = \hat{A} [\psi_\ell(r_1) \psi_m(r_2)] \quad (7)$$

The determination of the function $\psi_{Ei}(r_1, r_2)$ is assigned to the calculation of the coefficients $\Lambda_\mu(E)$ and $U_{ki}(E, r_2)$. Balashov et al., Senashenko et al., and Wague has stated Detailed calculation of these coefficients and systems of equations, respectively in [27-29]. Thus, the partial photoionization amplitude that describes the formation of a residual ion and a photoelectron in a definite state, has been defined by the following expression:

$$T_j = \langle \phi_j(E) | \hat{D} | \psi_0 \rangle + \frac{q+i}{\varepsilon-i} \langle \phi_\mu | \hat{V} | \phi_j(E) \rangle \frac{\sum_k \langle \phi_\mu | \hat{V} | \phi_k(E) \rangle \langle \phi_k(E) | \hat{D} | \psi_0 \rangle}{\sum_k |\langle \phi_\mu | \hat{V} | \phi_k(E) \rangle|^2} \quad (8)$$

In (7), $\phi_j(E)$ is the wave function of the continuous spectrum in the channel j , without resonance; $\varepsilon = (E - E_\mu) \frac{\Gamma_\mu^{\text{tot}}}{2}$ is the relative deviation from resonance; E_μ is the energy of the autoionisation level μ ; q is the profile index of the resonance; the sum of integrals in the denominator of (7) determines the total width of the autoionisation level μ

$$\Gamma_\mu^{\text{tot}} = 2\pi \sum_k |\langle \phi_\mu | \hat{V} | \phi_j(E) \rangle|^2 \quad (9)$$

3. Results and Discussion

Ordinary configuration states were performed $nln'l'$ to assess the double excited state by taking into consideration the mixing of the configurations. All the configurations contribute to the various decay channels and the predominant one in the doubly excited ($nln'l'$) L state can be highlighted using the eigenvectors.

On the basis of LS coupling scheme, 1^3P^o , 1^3D^o and 1^3F^o excitation energies throughout diagonalization calculations were performed, respectively, for 10, 16 and 17 configurations: $3ln'l'$ with $n' \leq 6$. We assigned respectively the basis on 16, 17, 19, 24 and 30 for the configurations ($4ln'l'$) with $n' \leq 7$, 1^3P^o , 1^3D^o , 1^3F^o , 1^3G^o and 1^3H^o autoionisation states.

Below the n threshold, the opened channels can be labeled $n_2l_2kl_1$; with n_2l_2 representing the state of the residual ion and $1/2k^2$ the energy of the ejected electron with angular momentum l_1 . The opened channels were based on the selection rules (conservation of L, S and the parity) which is responsible of the decay autoionisation states. For instance, the ($3ln'l'$) 1^3P^o resonance states has four decay channels, labeled 1skp, 2skp, 2pks, and 2pkd, which lead to N^{6+} in the indicated states 1s, 2s or 2p, an outgoing electron (in the k-shell) with the indicated angular momentum $l=0, 1, 2$.

By using the assumption that consists of neglecting the direct coupling between the opened channels, calculated partial autoionisation widths for n_2l_2 final sublevels are given in tables 1, 2 and 3 respectively for 1^3P^o , 1^3D^o and 1^3F^o ($3ln'l'$) doubly excited states of N^{5+} ions. In tables 4-8, autoionisation widths for n_2l_2 final sublevels of N^{6+} are also given for ($4ln'l'$): 1^3P^o , 1^3D^o , 1^3F^o , 1^3G^o and 1^3H^o states of N^{5+} . The value "0" in tables is to the respect of parity conservation, where the decay of sublevels or under the nearest ionizing threshold is forbidden. Due to the increasing of the accuracy base on the highest eigenvalues, selection was made on the right energies as we readapted the spectrum.

These include the calculation carried out by Bachau [26], who use a truncated diagonalization method to calculate $N=3$ resonances, Ho [30] and Ho with Bhatia [31]; they used a complex-coordinate rotation method.

The energy resonances calculations were in compliance with the theoretical results obtained by Bachau *and al.* [26], Ho [30], Ho and Bhatia [31] and Martin *and al.* [32].

the results related to the calculations of the partial widths ($3s3p$) 1^3P^o and ($3p3d$) 1^3P^o are in compliance with those obtained by Bachau *and al.*, Ho and Bhatia and Martin *and al.* as reported in table 1.

The partial widths calculated for 1^3D^o autoionisation states of the ion N^{5+} below the threshold $n=3$ reported in table 2, are not in compliance with those obtained by Bachau [26]. This discrepancy is due to the choice of the basis used.

The comparison of our total widths calculations of $4/4'$ singlet states with that of Ho [30], Ho and Bhatia [31] indicates a satisfactory agreement for the states ($4p4d$) 1^1P^o , ($4d4f$) 3^1P^o . The discrepancies noticed with the total width decay of ($4s4p$) 1^1P^o , ($4d4f$) 1^1P^o and ($4p4d$) 3^1P^o .

For the high values of the total angular momenta,

significant differences are found between our results and those found by Ho for the total widths of ($4d4f$) 3^1G^o and ($4d4f$) 1^1H^o reported in table 8. For these high values of the total angular momenta, the configuration interaction became stronger and the width calculation is more dependent to the choice of the wave functions.

The comparison of our values and those obtained by Bachau should not exhibit major discrepancies since we both used anti symmetrized product of hydrogenic orbitals for the double excited states, Coulomb wave function for the electron in the continuum and comparable dimensional basis set for the closed channel. The difference should be checked in the computational procedure.

The present calculations are expected to become more consistent, when high order coupling between the opened channels are taken into account.

Autoionisation leads preferentially to the nearest one-electron level of the residual ion; for the following, we will label this assumption rule 1. In some case, if the initial state is $nl_1n'l_2$, the preferred decay channel "reproduces" the angular momenta (l_1, l_2) of the initial configuration or that of the dominant configuration. In this case the autoionisation of the $nl_1n'l_2$ state leaves the residual ion with one of the initial angular momentum corresponding to the nearest one-electron level for e.g l_2 and then the leaving electron carrying the remaining angular momentum l_1 . For the following we will label this second assumption rule 2. (*see tables in appendix*)

In table 1, for energy, we noted a satisfactory agreement of our calculations with those Bachau [26] Ho and Bhatia [31] and Martin and al [32]. The two rules are both observed for partial widths of the triplet states ($3ln'l'$) 3^1P^o of N^{5+} ion. The state ($3s3p$) 3^1P^o decays preferentially towards $n_2l_2=2p$ excited state being the highest residual N^{6+} ion and electron ejected with the angular momentum $l_1=0$.

In table 2, we have a very satisfactory agreement among our energies calculated for 1^3D^o autoionization states of nitrogen ion N^{5+} sub threshold $n=3$ and the results obtained by Bachau [26]. Our partial widths calculated for 1^3D^o autoionisation states of the ion N^{5+} below the threshold $n=3$, disagree with those obtained by Bachau [26]. Rule 1 is observed in fact for all auto ionized states ($3ln'l'$) 1^3D^o which is leaving the residual ion in the 2p level, then can be consider as the highest excited level of residual ion in $n=3$.

Our energies reported in table 3, for 1^3F^o autoionisation states of nitrogen ion N^{5+} sub threshold $n=3$ are again in good compliance with the results obtained by Bachau [26]. The results obtained in the calculation of partial widths for autoionisation states 1^3F^o show compliance with the resonance ($4p3d$) 1^1F^o few correspondences for de-energizing to 2pkd channel and to a lesser extent to 2pkg.

The disintegration of states ($3ln'l'$) 1^3F^o N^{5+} ion, follows the first rule, leads to the state $n_2l_2=2p$ sublevels N^{6+} without conservation of angular momentum in the initial state or the predominant configuration.

For the results in table 4 the comparison with the results from Ho energies [30], shows a satisfactory agreement with the positions of resonances ($4ln'l'$) 1^3P^o .

The total widths are calculated by Ho only for the first three resonances $^{1,3}\text{P}^\circ$. Our results show discrepancies with those from Ho [30].

One can highlight that the states $(4ln'l')\ ^{1,3}P^\circ$ located above the threshold $n=3$ have additional decay channels $3skp$, $3pks$, $3pkd$, $3dkp$ and $3dkf$. The states $(4l4l')\ ^{1,3}P^\circ$ that are below the threshold $n=3$ have the same behavior as the states $(3ln'l')\ ^{1,3}P^\circ$. In fact, the rules 1 and 2 are both observed by the triplet $(4lnl')\ ^3P^\circ$ but the state $(4d4f)\ ^1P^\circ$ does not disintegrate preferentially to the highest excited state of the ion $2p$ residual N^{6+} .

For states $(4ln'l') \ ^1P^o$ which are located above the threshold $n=3$, none of the two rules is followed. The states $(4ln'l') \ ^3P^o$ located above the threshold $n=3$ is leaving residual N^{6+} ion in the excited state highest $2p$.

The values "0" indicated in table 4 for partial widths of states $(4lnl')^{1,3}P^o$ beneath the ionization threshold $n=3$ indicate that these states cannot auto ionized leaving residual ion in state $3s, 3p, 3d$ located above them.

In table 5, failing partial widths available in the literature, we compare our energy and total widths with those obtained by Ho and Bhatia [31] for states $(4ln'l')$ $^{1,3}\text{Do}$ N^{5+} ion above threshold $n=4$.

The states $(4ln'l') \ ^{1,3}D^o$ ion N^{5+} above threshold $n=3$ to disintegrate 2pkd channels 3pkd, 3dkp and 3dkf. The autoionization states $(4ln'l') \ ^1D^o$ preferentially under rule 2. The states $(4l4l') \ ^{1,3}D^o$, opened decay channels are reduced to the single 2pkd channel. The states $(4ln'l') \ ^3D^o$ that are below the threshold $n=3$ have the same behavior as the states $(3ln'l') \ ^{1,3}D^o$.

In the other hands, in table 6, we will simply compare our energy and total widths with those of Ho and Bhatia [31]. The correspondence between our energies and those of Ho and Bhatia is satisfactory but the results got for the total widths shows major concern.

These two references Ho and Bhatia allow us to assess as an asset of the sensitivity of the widths codes used. Indeed, in their work they used the same method with Hylleraas wave functions.

The states $(4ln'l')^1F^\circ$ of ion N^{5+} located below the threshold $n=3$ do not follow any of the two rules. They preferably disintegrate to $2s$. For the states $(4ln'l')^1F^\circ$ located above the

threshold $n=3$ none of the two rules is followed. Neither rules are observed by the states $(4ln'l')^3F^\circ$.

In table 7, we achieved good compliance between our energies and those obtained by Ho for resonances $(4\text{ln'l'}) } ^{1,3}\text{G}^\circ$. Regarding the two total widths calculated by Ho [30] on the first resonance $(4\text{d}4\text{f}) } ^1\text{G}^\circ$, it show any discrepancies with the results we have found.

The states $(4ln'l') \ ^{1,3}G^o$ of ion N^{5+} shown in table 7, decay channels have reduced due to conservation rule of parity (values "0" for the 1s and 2s states). The singlet states $(4ln'l') \ ^1G^o$ N^{5+} ion located above the threshold $n=3$ the following two rules; indeed, they auto ionized preferentially towards the channel 3dkf leaving residual ion in the excited state and the highest 3d ejected electron with angular momentum $l_1=3$. The states $(4ln'l') \ ^3G^o$ observe only the rule 1 and disintegrate preferences to $n_2l_2 \equiv 3d$.

In table 8, our energies calculated for the states $(4ln'l')^{1,3}H^\circ$ N^{5+} ion sub threshold $n=4$ are in very good agreement with those calculated by Ho [30]. Regarding the two total widths calculated by Ho there is a discrepancy with our results.

The states $(4n'l')\ ^{1,3}\text{H}^\circ$ of ion N^{5+} located below the threshold $n=3$ follow the rule 1 and auto ionized preferably through the 2pkg channel. As for the states $(4n'l')\ ^{1,3}\text{H}^\circ$ located above the threshold $n=3$, none of the two rules is respected.

4. Conclusion

In summary we have carried out the calculations of total and partial widths of the $(nln'l')^{1,3}L^o$ ($L=1, 2, 3, 4$ and 5) multiple-decay-channel system N^{5+} . From $L=1$ to 2 , the $(4l4l')^{1,3}L^o$ states located under $n=3$ and the $(3lnl')^{1,3}L^o$ states follow the same rules. All the $(4l4l')^{1,3}G^o$ and $(4l4l')^{1,3}H^o$ states located under $n=3$ observe the rule 1. None of the two rules are followed by the $(4lnl')^3F^o$ and $(4lnl')^{1,3}H^o$ states located above $n=3$. It worth noting that the behavior of the $(4lnl')^{1,3}F^o$ states is the same for states located under $n=3$ and those above $n=3$; for these states none of the rules is observed. Finally it is noticed that the rule 1 is the most frequent one. The results obtained here provide a proof of a dominance of the rule 1 in the $^{1,3}L^o$ autoionisation decay pathways.

Appendix

Table 1. Calculated energies $-E$, autoionisation width (eV), partial width (eV) and main configuration of the $1.3P^o$ states of the N^{5+} ion converging to $n=3$ hydrogen threshold.

[illegible]

states	−E(a.u)	Γ→1skp	Γ→2skp	Γ→2pks	Γ→2pkd	Γ→2p	Γ2s/Γ2p	Γ(Tot)
4p 3d ¹ P ^o	3,944 3,948 ^a	2,16[-3] 2,4[-3] ^a	7,14[-3] 7,2[-2] ^a	1,98[-2] 1,2[-1] ^a	4,04[-2] 4,3 [-2] ^a	6,03[-2] 1,63[-1] ^a	1,18[-1] 4,42[-1] ^a	6,96[-2] 2,4[-1] ^a
3p 4d ¹ P ^o	3,939 3,943 ^a	1,87[-3] 2,5[-4] ^a	8,06[-3] 6,2[-3] ^a	1,70[-3] 1,2[-2] ^a	9,01[-2] 1,2[-2] ^a	9,18[-2] 2,4[-2] ^a	8,78[-2] 2,58[-1] ^a	1,02[-1] 3,0[-2] ^a
3s 3p ³ P ^o	5,097 5,098 ^a 5,096 ^b	7,03[-4] 5,5[-4] ^a	5,88[-2] 3,8[-2] ^a	7,84[-2] 5,3[-2] ^a	1,41[-2] 1,3[-2] ^a	9,25[-2] 6,60[-2] ^a	6,36[-1] 5,76[-1] ^a	1,52[-1] 1,1[-1] ^a 1,05[-1] ^b
3p 3d ³ P ^o	5,098 ^c 5,096 ^d 4,910 4,915 ^a 4,914 ^c 4,911 ^d	4,85[-4] ^c 5,82[-4] ^d 7,24[-6] 2,3[-6] ^a 3,40[-7] ^c 2,39[-7] ^d	4,06[-2] ^c 4,24[-2] ^d 1,37[-2] 7,8[-3] ^a 7,74[-3] ^c 8,57[-3] ^d	5,38[-2] ^c 5,96[-2] ^d 1,70[-2] 1,2[-2] ^a 1,09[-2] ^c 1,39[-2] ^d	1,36[-2] ^c 1,44[-2] ^d 3,01[-2] 2,3[-2] ^a 2,42[-2] ^c 2,57[-2] ^d	6,74[-2] ^c 7,40[-2] ^d 4,72[-2] 3,5[-2] ^a 3,51[-2] ^c 3,96[-2] ^d	6,02[-1] ^c 5,72[-1] ^d 2,90[-1] 2,23[-1] ^a 2,20[-1] ^c 2,16[-1] ^d	1,08[-1] ^c 1,17[-1] ^d 6,08[-2] 4,3[-2] ^a 0,43[-1] ^c 0,48[-1] ^d
3s 4p ³ P ^o	3,997 3,998 ^a 3,997 ^b	6,18[-4] 2,8[-5] ^a	4,15[-2] 2,1[-4] ^a	6,06[-2] 9,5[-3] ^a	1,30[-2] 3,1[-6] ^a	7,37[-2] 9,5[-3] ^a	5,64[-1] 2,21[-2] ^a	1,16[-1] 9,7[-3] ^a
4s 3p ³ P ^o	3,992 3,997 ^a	1,00[-8] 4,1[-4] ^a	1,29[-5] 2,4[-2] ^a	1,48[-5] 2,7[-2] ^a	1,33[-4] 1,0[-2] ^a	1,48[-4] 3,70[-2] ^a	8,76[-2] 6,48[-1] ^a	1,60[-4] 6,2[-2] ^a
3p 4d ³ P ^o	3,889 3,892 ^a	6,07[-6] 1,8[-6] ^a	9,03[-3] 1,1[-3] ^a	1,01[-2] 8,2[-4] ^a	1,71[-2] 5,1[-3] ^a	2,72[-2] 5,92[-3] ^a	3,32[-1] 1,86[-1] ^a	3,62[-2] 7,0[-3] ^a

^a H. Bachau *and al.* [26].^cY. K. Ho and A. K. Bhatia [31].^dF Martin *and al.* [32].**Table 2.** Calculated energy resonances $-E$, autoionisation width (eV), partial width (eV) and main configuration of the $^{1,3}D^o$ states of the N^{5+} ion converging to $n=3$ hydrogen threshold.

states	−E(a.u)	Γ→1s	Γ→2s	Γ→2pks	Γ→2pkd	Γ→2p	Γ2s/Γ2p	Γ(Tot)
3p3d ¹ D ^o	4,944 5,005 ^a 5,004 ^c	0 0 ^a	0 0 ^a	0 0 ^a	7,36 [-2] 9,5 [-3] ^a	7,36 [-2] 9,5 [-3] ^a	0 0 ^a	7,36 [-2] 9,5 [-3] ^a 3,11[-4] ^c
4p3d ¹ D ^o	3,981 3,955 ^a 3,957 ^c	0 0 ^a	0 0 ^a	0 0 ^a	4,19 [-5] 2,3[-3] ^a	4,19 [-5] 2,3[-3] ^a	0 0 ^a	4,19 [-5] 2,3[-3] ^a 8,57[-5] ^c
3p4d ¹ D ^o	3,897 3,941 ^a 3,943 ^c	0 0 ^a	0 0 ^a	0 0 ^a	6,73 [-2] 4,3 [-3] ^a	6,73 [-2] 4,3 [-3] ^a	0 0 ^a	6,73 [-2] 4,3 [-3] ^a 1,44[-4] ^c
3d4f ¹ D ^o	3,833 3,869 ^a 3,869 ^c	0 0 ^a	0 0 ^a	0 0 ^a	1,27 [-3] 6,3 [-6] ^a	1,27 [-3] 6,3 [-6] ^a	0 0 ^a	1,27 [-3] 6,3 [-6] ^a 3,92[-7] ^c
5p3d ¹ D ^o	3,504 3,491 ^a 3,494 ^c	0 0 ^a	0 0 ^a	0 0 ^a	1,91[-3] 3,7[-3] ^a	1,91[-3] 3,7[-3] ^a	0 0 ^a	1,91 [-3] 3,7[-3] ^a 1,21[-4] ^c
3p3d ³ D ^o	5,003 4,944 ^a 4,945 ^c	0 0 ^a	0 0 ^a	0 0 ^a	2,16 [-2] 1,0[-1] ^a	2,16 [-2] 1,0[-1] ^a	0 0 ^a	2,16 [-2] 1,0[-1] ^a 3,96[-3] ^c
4p3d ³ D ^o	3,956 3,979 ^a 3,980 ^c	0 0 ^a	0 0 ^a	0 0 ^a	1,00 [-8] 1,1[-3] ^a	1,00 [-8] 1,1[-3] ^a	0 0 ^a	1,00 [-8] 1,1[-3] ^a 3,32[-5] ^c
3p4d ³ D ^o	3,937 3,902 ^a 3,903 ^c	0 0 ^a	0 0 ^a	0 0 ^a	9,96 [-3] 5,8[-2] ^a	9,96 [-3] 5,8[-2] ^a	0 0 ^a	9,96 [-3] 5,8[-2] ^a 2,16[-3] ^c
3d4f ³ D ^o	3,864 3,839 ^a 3,840 ^c	0 0 ^a	0 0 ^a	0 0 ^a	2,23 [-3] 4,9[-4] ^a	2,23 [-3] 4,9[-4] ^a	0 0 ^a	2,23 [-3] 4,9[-4] ^a 1,49[-5] ^c
3p5d ³ D ^o	3,489 3,502 ^a 3,505 ^c	0 0 ^a	0 0 ^a	0 0 ^a	7,33 [-3] 9,5 [-4] ^a	7,33 [-3] 9,5 [-4] ^a	0 0 ^a	7,33 [-3] 9,5 [-4] ^a 2,80[-5] ^c

^aH. Bachau *and al.* [26].^cY. K. Ho and A. K. Bhatia. [31].

Table 3. Calculated energy resonances $-E$, autoionisation width (eV), partial width (eV) and main configuration of the $^{1,3}F^o$ states of the N^{5+} ion converging to $n=3$ hydrogen threshold.

states	$-E(a.u)$	$\Gamma \rightarrow 1skf$	$\Gamma \rightarrow 2skf$	$\Gamma \rightarrow 2pkd$	$\Gamma \rightarrow 2pkg$	$\Gamma \rightarrow 2p$	$\Gamma 2s/\Gamma 2p$	$\Gamma(Tot)$
3p 3d $^1F^o$	4,845	1,59 [-4]	1,84 [-4]	3,38 [-3]	1,25 [-2]	1,58 [-2]	1,16 [-2]	8,98 [-2]
	4,848 ^a	2,2[-3] ^a	7,0[-2] ^a	2,5[-1] ^a	2,0[-2] ^a	2,70[-1] ^a	2,59[-1] ^a	3,5 [-1] ^a
	4,852 ^c							1,29[-2] ^c
3p 4d $^1F^o$	3,989	1,51 [-4]	5,47 [-4]	3,78 [-3]	6,77 [-3]	1,05 [-2]	5,19 [-2]	1,13 [-2]
	3,988 ^a	2,6 [-5] ^a	1,3[-3] ^a	5,0[-3] ^a	4,0[-5] ^a	5,04[-3] ^a	2,58[-1] ^a	6,3[-3] ^a
	3,989 ^c							2,02[-4] ^c
3d 4f $^1F^o$	3,902	2,95 [-5]	1,53 [-3]	5,46 [-3]	9,18 [-5]	5,55 [-3]	2,75 [-1]	7,44 [-2]
	3,906 ^a	2,7[-4] ^a	9,7 [-4] ^a	3,9 [-2] ^a	9,7[-5] ^a	3,91[-2] ^a	2,48[-2] ^a	4,0[-2] ^a
	3,907 ^c							1,41[-3] ^c
4p 3d $^1F^o$	3,841	1,93 [-3]	9,57 [-2]	1,33 [-1]	5,56 [-2]	1,89 [-1]	5,08 [-1]	2,87 [-1]
	3,852 ^a	1,2 [-3] ^a	3,9[-2] ^a	1,1[-1] ^a	2,2[-2] ^a	1,32[-1] ^a	2,95[-1] ^a	1,7[-1] ^a
	3,855 ^c							6,12[-3] ^c
3s 4f $^1F^o$	3,786	2,92 [-5]	1,49 [-3]	5,15 [-3]	9,82 [-5]	5,25 [-3]	2,85 [-1]	8,68 [-3]
	3,795 ^a	1,7[-4] ^a	7,8[-4] ^a	5,8[-3] ^a	3,5[-3] ^a	9,30[-3] ^a	8,39[-2] ^a	1,0[-2] ^a
	3,798 ^c							4,17[-4] ^c
3p 3d $^3F^o$	5,007	3,08 [-5]	3,08 [-3]	5,58 [-5]	7,51 [-3]	7,57 [-3]	4,07 [-1]	3,23 [-2]
	5,010 ^a	4,5[-4] ^a	7,0[-4] ^a	6,2[-5] ^a	4,0[-5] ^a	1,02[-4] ^a	6,86 ^a	1,2[-3] ^a
	5,008 ^b							4,09[-5] ^c
3p 4d $^3F^o$	3,944	2,75 [-5]	2,97 [-3]	2,51[-4]	2,39 [-3]	2,64 [-3]	1,12	5,64 [-3]
	3,950 ^a	3,5[-4] ^a	3,0[-4] ^a	1,8[-4] ^a	1,4[-5] ^a	1,94[-4] ^a	1,54	8,5[-4] ^a
	3,951 ^c							2,99[-5] ^c
4p 3d $^3F^o$	3,933	1,80 [-5]	1,01 [-3]	2,82 [-6]	4,11 [-4]	4,14 [-4]	2,43	1,14 [-2]
	3,935 ^a	1,3[-5] ^a	3,8[-6] ^a	1,5[-3] ^a	4,2[-4] ^a	1,92[-3] ^a	1,98[-3] ^a	1,9[-3] ^a
	3,935 ^c							8,24[-5] ^c
3d 4f $^3F^o$	3,912	4,17 [-4]	3,07 [-4]	5,74 [-4]	6,89 [-6]	5,81 [-4]	5,28 [-1]	3,54 [-3]
	3,915 ^a	8,2[-6] ^a	3,4[-3] ^a	8,3[-4] ^a	2,7[-3] ^a	3,53[-3] ^a	9,63[-1] ^a	7,0[-3] ^a
	3,915 ^c							3,08[-4] ^c
3s 4f $^3F^o$	3,858	4,15 [-4]	3,12 [-4]	4,72[-4]	7,84 [-6]	4,80 [-4]	6,49 [-1]	8,54 [-3]
	3,864 ^a	2,3[-5] ^a	2,6[-3] ^a	2,1[-4] ^a	1,3[-3] ^a	1,51[-3] ^a	1,72 ^a	4,1[-3] ^a
	3,865 ^c							1,60[-4] ^c

aH. Bachau and al. [26].

eA. K. Bhatia and Y. K. Ho [33].

Table 4. Calculated energy resonances $-E$, autoionisation width (eV), partial width (eV) and main configuration of the $^{1,3}P^o$ states of the N^{5+} ion converging to $n=4$ of N^{6+} .

States	$-E(a.u)$	$\Gamma \rightarrow 1skp$	$\Gamma \rightarrow 2skp$	$\Gamma \rightarrow 2pks$	$\Gamma \rightarrow 2pkd$	$\Gamma \rightarrow 3skp$	$\Gamma \rightarrow 3pks$	$\Gamma \rightarrow 3pkd$	$\Gamma \rightarrow 3dkp$	$\Gamma \rightarrow 3dkf$	$\Gamma(Tot)$
4s 4p $^1P^o$	2,853	3,93[-4]	1,66[-2]	2,28[-2]	8,77[-3]	0	0	0	0	0	4,86[-2]
	2,851 ^b										2,20[-1] ^b
4d 4f $^1P^o$	2,766	3,17[-4]	2,97[-5]	6,24[-6]	1,00[-3]	0	0	0	0	0	1,36[-3]
	2,765 ^b										6,52[-1] ^b
4p 4d $^1P^o$	2,594	1,29[-4]	4,13[-4]	1,03[-4]	3,96[-3]	7,89[-5]	3,94[-3]	2,09[-2]	3,75[-4]	6,74[-2]	9,73[-2]
	2,608 ^b										7,61[-2]
4s 5p $^1P^o$	2,380	3,99[-4]	1,47[-2]	2,15[-2]	9,67[-3]	3,00[-2]	4,28[-2]	6,55[-2]	5,57[-2]	1,01[-2]	2,50[-1]
4p 5d $^1P^o$	2,345	1,28[-4]	4,58[-4]	7,94[-5]	3,79[-3]	5,05[-4]	1,30[-3]	2,84[-2]	3,75[-5]	5,53[-2]	9,00[-2]
4s 4p $^3P^o$	2,880	9,78[-5]	4,32[-3]	7,46[-3]	1,84[-3]	0	0	0	0	0	1,37[-2]
	2,879 ^b										7,07[-2] ^b
4p 4d $^3P^o$	2,815	5,18[-6]	1,34[-3]	6,28[-4]	1,45[-3]	0	0	0	0	0	3,42[-3]
	2,813 ^b										2,14[-1] ^b
4d 4f $^3P^o$	2,708	5,00[-8]	1,18[-4]	2,34[-4]	1,08[-4]	8,36[-3]	9,27[-3]	2,08[-2]	8,20[-3]	2,59[-2]	7,30[-2]
	2,711 ^b										4,89[-2] ^b
4s 5p $^3P^o$	2,366	9,25[-5]	3,76[-3]	6,79[-3]	1,77[-3]	2,70[-2]	2,88[-2]	1,40[-2]	1,23[-2]	1,18[-3]	9,56[-2]
5s 4p $^3P^o$	2,360	4,00[-8]	3,00[-8]	2,00[-8]	4,60[-7]	1,94[-3]	1,40[-3]	2,91[-3]	3,58[-3]	1,87[-3]	1,17[-2]
5d 4f $^3P^o$	2,323	0	3,70[-6]	1,45[-5]	3,80[-7]	6,45[-4]	7,85[-4]	2,36[-4]	5,19[-4]	1,69[-4]	2,37[-3]

bY. K. Ho, Phys. Rev. A 35 [30].

Table 5. Calculated energy resonances $-E$, autoionisation width (eV), partial width (eV) and main configuration of the $^{1,3}D^o$ states of the N^{5+} ion converging to $n=4$ of N^{6+} .

states	$-E(a.u)$	$\Gamma \rightarrow 2s$	$\Gamma \rightarrow 2pkd$	$\Gamma \rightarrow 3pkd$	$\Gamma \rightarrow 3dkp$	$\Gamma \rightarrow 3dkf$	$\Gamma 2s/\Gamma 2p$	$\Gamma(Tot)$
4p 4d $^1D^o$	2,822	0	1,99[-3]	0	0	0	0	1,99[-3]
	2,845 ^c							4,78[-2]
4d 4f $^1D^o$	2,726	0	2,50[-3]	0	0	0	0	2,50[-3]
	2,767 ^c							8,59[-3] ^c
5p 4d $^1D^o$	2,361	0	4,73[-4]	1,59[-3]	1,20[-3]	1,96[-3]	0	5,23[-3]
	2,348 ^c							2,77[-3] ^c
5d 4f $^1D^o$	2,316	0	4,23[-6]	4,62[-4]	2,16[-4]	2,81[-4]	0	9,63[-4]
	2,337 ^c							3,10 [-2] ^c
4p 5d 1Do	2,314	0	1,79[-3]	6,32[-3]	2,00[-4]	6,65[-2]	0	7,48[-2]
	2,298 ^c							1,99[-3] ^c
4p 4d $^3D^o$	2,847	0	1,85[-6]	0	0	0	0	1,85[-6]
	2,820 ^c							1,05[-1] ^c
4d 4f $^3D^o$	2,766	0	1,45[-3]	0	0	0	0	1,45[-3]
	2,729 ^c							4,68[-2] ^c
5p 4d $^3D^o$	2,348	0	1,70[-7]	8,76[-6]	9,50[-7]	7,50[-5]	0	8,49[-5]
	2,360 ^c							1,75[-3] ^c
4p 5d $^3D^o$	2,335	0	9,00[-7]	4,96[-3]	2,04[-3]	7,59[-3]	0	1,46[-2]
	2,317 ^c							6,65[-2] ^c
5d 4f $^3D^o$	2,297	0	2,91[-5]	1,09[-3]	3,76[-5]	1,08[-3]	0	2,23[-3]
	2,314 ^c							4,52[-3] ^c

cY. K. Ho and A. K. Bhatia [31].

Table 6. Calculated energy resonances $-E$, autoionisation width (eV), partial width (eV) and main configuration of the $^{1,3}F^o$ states of the N^{5+} ion converging to $n=4$ of N^{6+} .

states	$-E(a.u)$	$\Gamma \rightarrow 1skf$	$\Gamma \rightarrow 2skf$	$\Gamma \rightarrow 2pkd$	$\Gamma \rightarrow 2pkg$	$\Gamma \rightarrow 3skf$	$\Gamma \rightarrow 3pkd$	$\Gamma \rightarrow 3pkg$	$\Gamma \rightarrow 3dkp$	$\Gamma \rightarrow 3dkf$	$\Gamma \rightarrow 3dkh$	$\Gamma(Tot)$
4s 4f $^1F^o$	2,822	6,37[-5]	8,18[-3]	1,82[-3]	4,42[-3]	0	0	0	0	0	0	1,69[-2]
	2,818 ^b											2,33[-1] ^b
	2,818 ^c											2,38[-1] ^c
	2,818 ^c											8,58[-3] ^c
4d 4f $^1F^o$	2,783	6,36[-5]	8,06[-3]	1,86[-3]	4,43[-3]	0	0	0	0	0	0	1,72[-2]
	2,784 ^b											3,16 [-1] ^b
	2,784 ^c											3,26 [-1] ^c
	2,784 ^c											1,16[-2] ^c
4p 4d $^1F^o$	2,667	1,92 [-4]	6,08[-4]	7,04[-3]	4,75[-4]	9,34[-2]	3,01[-2]	1,61[-2]	1,39[-5]	9,87[-2]	1,47[-2]	2,67[-1]
	2,672 ^b											2,59 [-1] ^b
	2,671 ^c											2,58 [-1] ^c
	2,672 ^c											9,53 [-3] ^c
5p 4d $^1F^o$	2,368	4,2[-7]	5,64[-5]	1,30[-4]	2,41[-4]	3,53[-3]	7,69[-4]	4,98[-3]	1,00[-3]	9,68[-3]	2,43[-4]	2,20[-2]
	2,368 ^c											3,66[-3] ^c
	2,368 ^c											1,34[-4] ^c
5s 4f $^1F^o$	2,336	3,57[-5]	5,77[-3]	6,33[-4]	2,96[-3]	1,65[-2]	5,37[-2]	1,93[-2]	2,97[-2]	3,37[-2]	2,03[-3]	2,39[-1]
	2,336 ^c											2,95 ^c
	2,336 ^c											1,08[-4] ^c
4p 4d $^3F^o$	2,858	7,02[-5]	4,41[-5]	3,40[-7]	3,70[-7]	0	0	0	0	0	0	2,15[-4]
	2,855 ^b											9,20[-2] ^b
	2,855 ^c											3,38[-3] ^c
4d 4f $^3F^o$	2,805	2,37[-6]	5,37[-4]	3,27[-4]	7,74[-4]	0	0	0	0	0	0	3,09[-3]
	2,805 ^b											4,14[-2] ^b
	2,805 ^c											3,94[-2] ^c
	2,805 ^c											1,52[-3] ^c
4s 4f $^3F^o$	2,767	2,36[-6]	5,24[-4]	3,22[-4]	7,67[-4]	0	0	0	0	0	0	1,70[-3]
	2,767 ^b											7,84[-3] ^b
	2,767 ^c											2,72[-3] ^c
	2,767 ^c											2,88[-4] ^c
5p 4d $^3F^o$	2,349	1,8[-7]	1,10[-4]	2,41[-5]	6,49[-5]	4,20[-3]	1,80[-3]	2,41[-3]	5,65[-4]	2,64[-3]	2,13[-4]	2,67[-2]
	2,349 ^c											5,52[-3] ^c
	2,349 ^c											2,03[-4] ^c
4p 5d $^3F^o$	2,344	6,60[-5]	5,32[-5]	3,80[-5]	1,72[-6]	8,17[-3]	4,21[-2]	1,07[-3]	5,66[-2]	1,42[-3]	5,29[-5]	1,12[-1]
	2,346 ^c											5,67[-2] ^c
	2,346 ^c											2,08[-3] ^c

bY. K. Ho, Phys. Rev. A 35 [30].

cY. K. Ho and A. K. Bhatia [31].

cA. K. Bhatia and Y. K. Ho [33].

Table 7. Calculated energy resonances $-E$, autoionisation width (eV), partial width (eV) and main configuration of the $^{1,3}G^o$ states of the N^{5+} ion converging to $n=4$ of N^{6+} .

states	$-E(a.u)$	$\Gamma \rightarrow 1s$	$\Gamma \rightarrow 2s$	$\Gamma \rightarrow 2pkg$	$\Gamma \rightarrow 3pkg$	$\Gamma \rightarrow 3dkf$	$\Gamma \rightarrow 3dkh$	$\Gamma 2s/\Gamma 2p$	$\Gamma(Tot)$
4d 4f $^1G^o$	2,762	0	0	2,71[-3]	0	0	0	0	2,71[-3]
	2,762 ^b								5,71[-3] ^b
4p 5g $^1G^o$	2,336	0	0	3,13[-4]	1,99[-3]	2,32[-2]	1,02[-3]	0	2,65[-2]
5d 4f $^1G^o$	2,303	0	0	1,06[-3]	1,97[-2]	2,92[-2]	9,48[-3]	0	5,94[-2]
4d 5f $^1G^o$	2,274	0	0	2,38[-3]	2,30[-2]	8,95[-2]	7,68[-3]	0	1,22[-1]
4f 5g $^1G^o$	2,243	0	0	3,05[-4]	1,89[-3]	2,25[-2]	9,91[-4]	0	2,56[-2]
4d 4f $^3G^o$	2,804	0	0	3,05[-4]	0	0	0	0	3,05[-4]
	2,804 ^b								2,02 ^b
4d 5f $^3G^o$	2,317	0	0	2,40[-4]	9,49[-4]	3,65[-3]	4,66[-4]	0	5,31[-3]
5d 4f $^3G^o$	2,311	0	0	3,34[-5]	3,45[-3]	9,11[-4]	5,60[-3]	0	9,99[-3]
4p 5g $^3G^o$	2,302	0	0	6,36[-4]	3,90[-4]	5,20[-5]	8,33[-4]	0	1,91[-3]
4f 5g $^3G^o$	2,277	0	0	6,27[-4]	4,06[-4]	9,16[-5]	8,29[-4]	0	1,95[-3]

bY. K. Ho, Phys. Rev. A 35 [30].

Table 8. Calculated energy resonances $-E$, autoionisation width (eV), partial width (eV) and main configuration of the $^{1,3}H^o$ states of the N^{5+} ion converging to $n=4$ of N^{6+} .

states	$-E(a.u)$	$\Gamma \rightarrow 1skh$	$\Gamma \rightarrow 2skh$	$\Gamma \rightarrow 2pkg$	$\Gamma \rightarrow 2pki$	$\Gamma \rightarrow 3skh$	$\Gamma \rightarrow 3pkg$	$\Gamma \rightarrow 3pki$	$\Gamma \rightarrow 3dkf$	$\Gamma \rightarrow 3dkh$	$\Gamma \rightarrow 3dkj$	$\Gamma(Tot)$
4d 4f $^1H^o$	2,713	7,00[-8]	3,51[-4]	7,74[-4]	5,08[-5]	2,69[-4]	7,53[-3]	1,40[-5]	2,75[-2]	3,67[-5]	1,30[-7]	3,96[-2]
	2,716 ^b											6,66[-1] ^b
	2,337	6,00[-8]	3,40[-4]	6,87[-4]	5,56[-5]	3,97[-4]	5,32[-3]	4,23[-5]	1,44[-2]	1,84[-4]	1,02[-6]	4,82[-2]
4f 5g $^1H^o$	2,283	3,85[-6]	8,99[-4]	9,79[-3]	3,00[-8]	6,61[-2]	1,18[-1]	1,45[-2]	1,65[-1]	4,86[-2]	7,72[-4]	4,84[-1]
5d 4f $^1H^o$	2,245	2,33[-6]	4,17[-4]	6,37[-3]	5,52[-5]	1,44[-1]	2,04[-1]	2,60[-2]	1,07[-1]	1,35[-1]	4,60[-4]	7,46[-1]
4p 5g $^1H^o$	2,213	3,83[-6]	9,33[-4]	9,70[-3]	4,00[-8]	6,60[-2]	1,03[-1]	1,60[-2]	1,68[-1]	4,67[-2]	9,39[-4]	4,37[-1]
4d 4f $^3H^o$	2,800	1,20[-7]	2,71[-4]	4,42[-4]	9,05[-5]	0	0	0	0	0	0	1,21[-3]
	2,800 ^b											2,72[-2] ^b
4f 5g $^3H^o$	2,310	1,70[-7]	2,93[-5]	1,06[-4]	3,96[-5]	7,10[-7]	4,38[-3]	9,10[-5]	7,67[-4]	8,44[-3]	1,74[-5]	1,92[-2]
4d 5f $^3H^o$	2,304	1,20[-7]	2,13[-4]	2,90[-4]	8,39[-5]	1,29[-4]	2,08[-4]	2,10[-4]	5,86[-3]	9,92[-3]	2,10[-5]	2,69[-2]
5d 4f $^3H^o$	2,294	3,00[-8]	1,54[-4]	4,00[-7]	1,01[-4]	7,16[-4]	7,03[-3]	1,28[-4]	1,08[-3]	1,85[-2]	8,00[-8]	2,97[-2]
4p 5g $^3H^o$	2,270	1,70[-7]	2,79[-5]	1,04[-4]	3,87[-5]	2,00[-8]	4,02[-3]	9,98[-5]	6,61[-4]	7,94[-3]	1,94[-5]	1,49[-2]
4d 6f $^3H^o$	2,066	1,10[-7]	1,89[-4]	2,37[-4]	8,03[-5]	1,61[-4]	6,70[-7]	2,97[-4]	8,07[-3]	7,51[-3]	3,74[-5]	2,05[-2]

b Y. K. Ho, Phys. Rev. A 35 [30].

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