The theoretical calculation of transition probabilities for some excited p-d transitions in atomic nitrogen

G. Çelik^a, E. Akın, and H.Ş. Kılıç

Department of Physics, Faculty of Arts and Science, Selçuk University, Campus 42075 Konya, Turkey

Received 19 March 2006 / Received in final form 13 June 2006 Published online 28 July 2006 – © EDP Sciences, Società Italiana di Fisica, Springer-Verlag 2006

Abstract. The atomic transition probabilities are calculated for individual lines between some quartet terms of $3p \rightarrow 4d$ and $3p \rightarrow 5d$ transition arrays using weakest bound electron potential model theory (WBEPMT). In the determination of relevant parameters which are needed for calculation of transition probabilities, we employed numerical non-relativistic Hartree-Fock wave functions for expectation values of radius in both ground and excited states unlike to NCA method used on traditional WBEPMT procedure. We have obtained very good agreement between our results and the accepted values taken from NIST.

PACS. 31.10.+z Theory of electronic structure, electronic transitions, and chemical binding – 32.70.Cs Oscillator strengths, lifetimes, transition moments

1 Introduction

The determination of physical properties of nitrogen are very important in both astrophysics and atmosphere science. Absorption lines observed in sun light related to the transitions between fine structure levels may contain very important information about far stars in galaxy. On the other hand, the amount of nitrogen at stars can be determined depending on the atomic transition probabilities [1,2]. One of the most important parameters in the atomic spectroscopy is the transition probability. The obtained values for the transition probabilities include some important information about the selection of relevant transitions, temperature and atomic concentrations. Many studies have been carried out to determine the transition probabilities and oscillator strengths theoretically in nitrogen atom. Beck and Nicolaides have calculated the oscillator strengths for the atomic nitrogen and oxygen. They applied a combination of the Multi-Configurational Hartree-Fock (MCHF) method with Variational Configuration-Interaction (VCI) calculations [3]. Fawcet has calculated oscillator strengths for N II using relativistic HF technique [4]. Hofsaess has calculated term energy levels and oscillator strengths for nitrogen by the Thomas-Fermi-Hartree-Fock method (TFHF) [5]. Suskin and Weiss have studied the correlation effects within quartet states of nitrogen using a CI expansion of approximately 3000 configurations [6]. Bell and Berrington have calculated oscillator strengths and photo-ionization cross-sections for atomic nitrogen using

R-Matrix method in the LS coupling [7]. Hibbert et al. have calculated the transition probabilities for individual lines using the configuration-interaction version 3 (CIV3) code based on configuration interaction wave functions [8]. Tong et al. have calculated the oscillator strengths of electric-dipole allowed transitions among the low-lying states of quartet symmetry in atomic nitrogen using MCHF procedure [9]. Energy levels and transitions in N II have been studied by Fischer using MCHF approximation [10]. Bell et al. have calculated the transition probabilities for transitions between the some fine structure levels of singly ionized nitrogen using configuration interaction wave functions and the CIV3 code [11]. Robinson and Hibbert have studied the transitions from the ground state to the four lowest ⁴P states with the CIVNON code using a restricted the non-orthogonal representation for both the lower and upper states [12]. Zheng-Wang and Zheng et al. have calculated resonance transition probabilities for transitions between several levels and lifetimes for some excited states using WBEPMT on the atomic and ionic nitrogen [13,14]. The results obtained from Breit-Pauli approximation for energy levels, lifetimes and Landé q(J) factors have been determined for all levels up to 2p(2)3d in the nitrogen-like sequence (Z = 7-17)and 2p(3)3d in the oxygen-like sequence (Z = 8-20) by Tachiev and Fischer [15].

In this study, we employed WBEPM theory for the calculations of transition probabilities of some excited p-d transitions in atomic nitrogen. This theory uses the observed binding energy and expectation values of radius to find the effective values of nuclear charge, principal quantum number and orbital quantum number. These

^a e-mail: gultekin@selcuk.edu.tr

parameters then define the radial function of the weakest bound electron. This method has a simple calculation procedure. Moreover, the determination of Z^* , n^* and l^* parameters is sufficient for the calculation of transition probabilities. In this work, we have used the numerical non-relativistic Hartree-Fock wave functions for determination of relevant parameters and then atomic transition probabilities calculated in framework of WBEPM theory.

2 Theory and calculation procedure

The weakest bound electron potential model theory (WBEPMT) has been development by Zheng [16]. He was suggested a new model potential to describe the electronic motion in a multi-electron atomic or ionic systems and separated into two groups of electrons to be the weakest bound electron and non-weakest bound electrons in given a system. As viewed from excitation or ionization procedures, the weakest bound electron in an atom or ion differs from other electrons in the behavior. The weakest bound electron (WBE) in many-electron systems is that electron most weakly bound to the system compared to the other electrons in the system. Some atomic or ionic properties in a multi-electron systems such as transition, excitation and ionization may be referred to weakest bound electron's behavior. Therefore, the weakest bound electron in a given atomic or ionic system is also the electron which can most easily be excited or ionized. Accurate treatment of WBE can obtained accurate information about these properties. By the separation of the electrons in a given system, complex many-electron problem can be simplified as the single electron problem and so can be solve easily [17-20].

According to WBEPM theory, the Schrödinger equation of the weakest bound electron in under nonrelativistic conditions (in a.u.) given as [23]

$$-\frac{1}{2}\nabla^2\psi_i + V(r_i)\psi_i = \varepsilon_i\psi_i \tag{1}$$

$$V(r_i) = -\frac{Z^*}{r_i} + \frac{[d(d+1) + 2dl]}{2r_i^2}.$$
 (2)

Here $V(r_i)$ is potential function produced by the nonweakest bound electrons and nucleus. Screening by the non-weakest bound electron is not complete because of the orbital penetration effect of the weakest bound electron. The nuclear charge acting on the WBE would be an effective nuclear charge Z^* which is non-integer. However, l is the angular momentum quantum number of the weakest bound electron and d is an undetermined parameter. Moreover, the principal quantum number n and angular quantum number l of the weakest bound electron replaced by the effective principal quantum number n^* and effective angular momentum quantum number l^* . In WBEPM theory, weakest bound electron is move in a central potential. Potential function can be divided into two parts. The first term is Coulomb potential related to the penetration and screening effect and second term is the dipole potential produced by polarization effect. Using this new

model potential, the electronic radial wave function can be expressed by means of general Laguerre polynomial with parameters determined from experimental ionization data [20].

The wave function of the weakest bound electron can be given as

$$\psi_i(r_i, \theta_i, \varphi_i) = R_{n^*l^*}(r_i) Y_{l,m}(\theta_i, \varphi_i)$$
(3)

where, $Y_{l,m}(\theta_i,\varphi_i)$ is complex spherical harmonics and $R_{n^*l^*}(r_i)$ is radial parts of wave function. Substituting this potential function into the Schrödinger equation of the weakest bound electron and solving the radial equation by employing some transformations, the radial wave function of the weakest bound electron [19,23] can be obtained to be

$$R_{n^*l^*}(r) = C \exp\left(-\frac{Z^*r}{n^*}\right) r^{l^*} L_{n^*-l^*-1}^{2l^*+1}\left(\frac{2Z^*r}{n^*}\right)$$
(4)

where $L_{n^*-l^*-1}^{2l^*+1}(2Z^*r/n^*)$ is the general Laguerre polynomial and C is normalization constant given to be

$$C = \left(\frac{2Z^*}{n^*}\right)^{l^*+3/2} \left[\frac{2n^*}{(n^*-l^*-1)!} \Gamma\left(n^*-l^*+1\right)\right]^{-1/2}.$$
(5)

The energy eigenvalue of the weakest bound electron given as

$$\varepsilon = -\frac{Z^{*^2}}{2n^{*^2}}.$$
(6)

Here, n^* and l^* parameters have been given to be

$$l^* = l + d \tag{7}$$

$$n^* = n + d. \tag{8}$$

The negative value of the energy ε in equation (6) may be set approximately equal to the binding energy of the spectroscopic energy level of the WBE,

$$E = \varepsilon = -\frac{Z^{*^2}}{2n^{*^2}} \tag{9}$$

where, E can be obtained from the experimental excitation spectral energy level E_{spec} and spectral limit value $E_{\lim it}$,

$$E = E_{\lim it} - E_{spec}.$$
 (10)

In WBEPM theory, radial transition integral has been determined using radial wave function given in equation (4) and integral formula of two generalized Laguerre polynomials given to be

$$\int_{0}^{\infty} t^{\lambda} e^{-t} L_{m}^{\mu}(t) L_{m'}^{\mu'}(t) dt = (-1)^{m+m'} \Gamma(\lambda+1)$$
$$\times \sum_{k} {\binom{\lambda-\mu}{m-k} \binom{\lambda-\mu'}{m'-k} \binom{\lambda+k}{k}} (11)$$

$$\langle n_i, l_i | r^k | n_f, l_f \rangle = \int_0^\infty r^{k+2} R_{n_i l_i}(r) R_{n_f l_f}(r) dr = (-1)^{n_f + n_i + l_f + l_i} \left(\frac{2Z_f^*}{n_f^*} \right)^{l_f^*} \left(\frac{2Z_i^*}{n_i^*} \right)^{l_i^*} \left(\frac{Z_f^*}{n_f^*} - \frac{Z_i^*}{n_i^*} \right)^{-l_f^* - l_i^* - k - 3} \left[\frac{n_f^{*4} \Gamma(n_f^* + l_f^* + 1)}{4Z_f^{*3} (n_f - l_f - 1)!} \right]^{-1/2} \times \left[\frac{n_i^{*4} \Gamma(n_i^* + l_i^* + 1)}{4Z_i^{*3} (n_i - l_i - 1)!} \right]^{-1/2} \sum_{m_1 = 0}^{n_f - l_f^* - 1} \sum_{m_2 = 0}^{n_i - l_i^* - 1} \frac{(-1)^{m_2}}{m_1! m_2!} \left(\frac{Z_f^*}{n_f^*} - \frac{Z_i^*}{n_i^*} \right)^{m_1 + m_2} \times \left(\frac{Z_f^*}{n_f^*} + \frac{Z_i^*}{n_i^*} \right)^{-m_1 - m_2} \Gamma(l_f^* + l_i^* + m_1 + m_2 + k + 3) \times \sum_{m_3 = 0}^{S} \left(l_i^* - l_f^* + k + m_2 + 1 \\ n_f^* - l_f^* - 1 - m_1 - m_3 \right) \left(l_f^* - l_i^* + k + m_1 + 1 \\ n_i^* - l_i^* - 1 - m_2 - m_3 \right) \left(l_i^* + l_f^* + k + m_1 + m_2 + m_3 + 2 \\ m_3 \right)$$
(12)

where, the quantities under the integral sign are in the form of $t = (Z_1^*/n_1^* + Z_2^*/n_2^*)r$,

$$\lambda = l_1^* + l_2^* + k + 2, \quad m = n_1 - l_1 - 1,$$

$$m' = n_2 - l_2 - 1, \qquad \mu = 2l_1^* + 1, \qquad \mu' = 2l_2^* + 1.$$

Then, for a transition from the level (n_i, l_i) to the level (n_f, l_f) , the expectation value of r^k or radial transition integral for k = 1 is given to be [19,23–26]

where $S = \min\{n_f^* - l_f^* - 1 - m_1, n_i^* - l_i^* - 1 - m_2\}$ and $k > -l_f^* - l_i^* - 3$ if k = 1 and f = i, expectation value of the weakest bound electron i can be written

$$\langle r \rangle = \frac{3n^{*^2} - l^*(l^* + 1)}{2Z^*}.$$
 (13)

In order to calculate ε , R and other properties of the WBE, the parameters Z^* and d are must be known and so the equations (9) and (13) must be solved together. It is well-known that some difficulties in obtaining the parameters directly from theory are still present. Therefore, Zheng suggest that the values of E_{spec} can be taken from the experimental atomic data in the literature and expectation value of radius of the weakest bound electron $\langle r \rangle$ can be obtained by many theoretical methods such as Numerical Coulomb Approximation (NCA), Multiconfigurational Hartree-Fock (MCHF) method, Roothaan-Hartree-Fock (RHF) Method, Hartree-Kohn-Sham Method (HKS), time-dependent Hartree-Fock (TDHF) etc. [20, 22]. In this study, expectation values of radius of the weakest bound electron for all levels have determined from Hartree-Fock Method. We employed HF96 computer program based on the numerical non-relativistic wave functions. In this package program, numerical non-relativistic Hartree-Fock wave functions are determined for atoms. These wave functions are used to predict a variety of atomic parameters as Slater and magnetic integrals, spin-orbit parameters, electron density at the nucleus and transition integrals [27,28].

Electric dipole transition probability from a state to other has been given as following

$$A = \frac{64\pi^4 e^2 a_0^2 (E_{J'} - E_j)^3}{3h(2J' + 1)} S.$$
 (14)

Here, $(E_j - E_i)$ is the energy difference between relevant levels and S is the electric dipole line strength [29]. Line strength is determined according to the coupling schemes and the transition types in atomic or ionic systems. The text book given by Cowan [29] has presented in details how the line strength can be calculated due to considered coupling schemes and for different type transitions.

According to the weakest bound electron potential model theory, in the calculation of transition probabilities for atomic nitrogen, the determination of Z^* and d parameters is sufficient. In the determination of these parameters, equations (9) and (13) solved together. Energy values used in equation (9) are taken from experimental values in the literature [30] and expectation values of radius for ground and excited levels are calculated using Hartree-Fock method [27,28]. The parameters required for the calculations of the transition probabilities have been determined using the procedure mentioned above and presented in Table 1.

3 Results and conclusions

We have calculated atomic transition probabilities for individual lines between some quartet terms of $3p \rightarrow 4d$ and $3p \rightarrow 5d$ transition arrays using WBEPM theory in nitrogen atom. We employed numerical nonrelativistic Hartree-Fock wave functions for expectation values of radius in both ground and excited states which is used in determination of relevant parameters. Available experimental and theoretical data are quite limited for this spectrum. On the other hand these data have not been sensitively tested for both the multiplet values and for the individual lines. Therefore, the results obtained from our calculation have been compared to only extensive database of transition probabilities taken from NIST [32].

Table 1. The parameters for the calculations of transition probabilities.

Level	n	l	d	Z^*	$\langle r \rangle$	Energy (cm^{-1})
$1s^2 2s^2 2p^2$ (³ P) $3p^4 P_{1/2}$	3	1	-0.912676	0.929278	6.981652	21750.39
$1s^2 2s^2 2p^2$ (³ P) $3p$ ⁴ P _{3/2}	3	1	-0.913745	0.928410	6.981652	21732.01
$1s^2 2s^2 2p^2$ (³ P) $3p$ ⁴ P _{5/2}	3	1	-0.915981	0.926594	6.981652	21693,55
$1s^2 2s^2 2p^2$ (³ P) $3p$ ⁴ D _{1/2}	3	1	-0.939026	0.932288	6.799479	22454.82
$1s^2 2s^2 2p^2$ (³ P) $3p$ ⁴ D _{3/2}	3	1	-0.940279	0.931251	6.799479	22432.21
$1s^2 2s^2 2p^2$ (³ P) $3p^4 D_{5/2}$	3	1	-0.942354	0.929538	6.799479	22394.81
$1s^2 2s^2 2p^2$ (³ P) $3p^4 D_{7/2}$	3	1	-0.945180	0.927205	6.799479	22343.88
$1s^2 2s^2 2p^2$ (³ P) $4p \ ^4P_{1/2}$	4	1	-0.831999	0.967985	15.450882	10245.22
$1s^2 2s^2 2p^2$ (³ P) $4p \ ^4P_{3/2}$	4	1	-0.834758	0.966408	15.450882	10229.66
$1s^2 2s^2 2p^2$ (³ P) $4p \ ^4P_{5/2}$	4	1	-0.842043	0.962247	15.450882	10188.63
$1s^2 2s^2 2p^2$ (³ P) 4d ⁴ P _{1/2}	4	2	-0.082247	0.980658	20.624307	6075.686
$1s^2 2s^2 2p^2$ (³ P) 4d ⁴ P _{3/2}	4	2	-0.072636	0.958013	20.624307	6902.979
$1s^2 2s^2 2p^2$ (³ P) 4d ⁴ P _{5/2}	4	2	-0.064638	0.988644	20.624307	6925.726
$1s^2 2s^2 2p^2$ (³ P) 4d ⁴ D _{1/2}	4	2	-0.016580	0.994498	20.958065	6839.905
$1s^2 2s^2 2p^2$ (³ P) 4d ⁴ D _{3/2}	4	2	-0.020060	0.992927	20.958065	6830.237
$1s^2 2s^2 2p^2$ (³ P) 4d ⁴ D _{5/2}	4	2	-0.022182	0.991969	20.958065	6824.344
$1s^2 2s^2 2p^2$ (³ P) 4d ⁴ D _{7/2}	4	2	-0.022850	0.991666	20.958065	6822.48
$1s^2 2s^2 2p^2$ (³ P) $5d^4 D_{1/2}$	5	2	-0.060172	0.980250	34.431473	4321.20
$1s^2 2s^2 2p^2$ (³ P) $5d {}^4D_{3/2}$	5	2	-0.063395	0.979092	34.431473	4316.62
$1s^2 2s^2 2p^2$ (³ P) $5d^4 D_{5/2}$	5	2	-0.064489	0.978698	34.431473	4315.07
$1s^2 2s^2 2p^2$ (³ P) $5d^4 D_{7/2}$	5	2	-0.064805	0.978585	34.431473	4314.62
$1s^2 2s^2 2p^2$ (³ P) $5d {}^4F_{3/2}$	5	2	-0.046656	0.999235	33.944920	4465.73
$1s^2 2s^2 2p^2$ (³ P) $5d^4 F_{5/2}$	5	2	-0.046901	0.999146	33.944920	4465.375
$1s^2 2s^2 2p^2$ (³ P) $5d^4 F_{7/2}$	5	2	-0.072491	0.989812	33.944920	4427.975
$1s^2 2s^2 2p^2$ (³ P) $5d^4 F_{9/2}$	5	2	-0.011620	0.973958	33.944920	4364.352
$1s^2 2s^2 2p^2$ (³ P) $5d^4 P_{1/2}$	5	2	-0.036108	0.988919	34.027040	4355.43
$1s^2 2s^2 2p^2$ (³ P) $5d$ ⁴ P _{3/2}	5	2	-0.013499	0.997094	34.027040	4387.68
$1s^2 2s^2 2p^2$ (³ P) $5d$ ⁴ P _{5/2}	5	2	-0.004011	1.000534	34.027040	4401.24

The NIST is a database of accepted values and collect accepted data from the original sources where original data obtained from theoretical and/or experimental works. So, the NIST contains recommended values for many transitions taken from original sources as well. The values collected by NIST database are known to be the best available data at that time. Our data presented in comparison with accepted NIST data followed by its accuracy rating in fifth column of Table 2. It has been seen from Table 2 that the data calculated in this work presents a good agreement with the accepted values within given their uncertainty rates.

Zheng et al. have used the WBEPM theory for the determination of some important physical parameters such as energy levels, ionization potentials, transition probabilities, oscillator strengths and lifetimes. They have preferred Numerical Coulomb Approximation (NCA) for the expectation values of radius which is used in determination of relevant parameters. In the NCA method, for the ground state and some excited states, the deviation between real expectation values and values calculated from NCA method is very large [13,19,31]. In our paper, we have used the HF96 computer program [28] based on the numerical non-relativistic wave functions instead of NCA method which is commonly employed in the studies using WBEPMT in the literature for expected values of radius. We have obtained very good agreement between our results and the accepted values taken from NIST.

The Configuration Interaction (CI) and MCHF methods are powerful methods taken into account the relativistic and correlation effects. In the CI approximation many configurations are required to obtain more accurate results, especially more configurations must be considered for the excited states of many-electron systems and it causes the calculation become very complicated. In the MCHF approximations, atomic wave functions are obtained using many basis-set orbital functions. The reliability and accuracy of the results depend on the number of the basis-set orbital functions chosen. It is difficult to deal with many configuration and orbital basis set functions and not practicable in calculations. The study of highly excited states and highly ionized states of atoms using well-known ab-initio methods are also very difficult. Therefore, theoretical works in the literature have been limited to the lower excited levels. For example, CI and MCHF results contain data only for the transitions up to 4s and 3d levels. In atomic nitrogen, there are five electrons apart from the $1s^2$ core electron. It is not easy to deal with high lying levels excited of these multi-electron systems using well-known standard methods. In this work, we have obtained the transition probabilities between individuals lines of atomic nitrogen in the higher excited

Transitions	This work $(\times 10^8 \text{ sn}^{-1})$	Accepted values (Ref. [32])	Accuracy [*] (Ref. [32])
$1s^2 2s^2 2p^2 ({}^{3}P) 3p {}^{4}P_{1/2} \rightarrow 1s^2 2s^2 2p^2 ({}^{3}P) 4d {}^{4}P_{1/2}$	0.00210	0.00195	D+
$1s^2 2s^2 2p^2 ({}^{3}P) 3p {}^{4}P_{3/2} \rightarrow 1s^2 2s^2 2p^2 ({}^{3}P) 4d {}^{4}P_{1/2}$	0.00960	0.00973	D+
$1s^2 2s^2 2p^2 ({}^{3}P) 3p {}^{4}P_{1/2} \rightarrow 1s^2 2s^2 2p^2 ({}^{3}P) 4d {}^{4}P_{3/2}$	0.00488	0.00485	D+
$1s^2 2s^2 2p^2 ({}^{3}P) 3p {}^{4}P_{3/2} \rightarrow 1s^2 2s^2 2p^2 ({}^{3}P) 4d {}^{4}P_{3/2}$	0.00155	0.00155	D+
$1s^2 2s^2 2p^2 ({}^{3}P) 3p {}^{4}P_{3/2} \rightarrow 1s^2 2s^2 2p^2 ({}^{3}P) 4d {}^{4}P_{5/2}$	0.00350	0.00347	D+
$1s^2 2s^2 2p^2 ({}^{3}P) 3p {}^{4}P_{5/2} \rightarrow 1s^2 2s^2 2p^2 ({}^{3}P) 4d {}^{4}P_{3/2}$	0.00517	0.00518	D+
$1s^2 2s^2 2p^2$ (³ P) $3p^{-4} P_{5/2} \rightarrow 1s^2 2s^2 2p^2$ (³ P) $4d^{-4} P_{5/2}$	0.00806	0.00802	D+
$1^{2}_{2}^{2}_{2}^{2}_{2}^{2}_{3}^{(3)}_{2}^{2}_{3}^{(3)}_{2}^{2}_{4}^{(3)}_{2}^{2}_{2}^{(3)}_{2}^{(3)}_{2}^{(3)}_{4}^{(4)}_{4}^{4}_{7}^{7}_{7}^{1}_{2}^{2}_{2}^{2}_{2}^{2}_{2}^{(3)}_{2}^{(3)}_{2}^{(3)}_{4}^{(4)}_{4}^{4}_{7}^{7}_{7}^{1}_{2}^{2}_{2}^{2}_{2}^{2}_{2}^{(3)}_{2}^{(3)}_{2}^{(3)}_{2}^{(4)}_{2}^$	0.00600	0.00700	C
$1s^{-}2s^{-}2p^{-}({}^{\circ}P) 3p^{-}D_{1/2} \rightarrow 1s^{-}2s^{-}2p^{-}({}^{\circ}P) 4d^{-}D_{1/2}$ $1s^{-}2s^{-}2p^{-}({}^{\circ}P) 4d^{-}D_{1/2} \rightarrow 1s^{-}2s^{-}2p^{-}({}^{\circ}P) 4d^{-}D_{1/2}$	0.00628	0.00789	C
$1s \ 2s \ 2p \ (P) \ 3p \ D_{1/2} \rightarrow 1s \ 2s \ 2p \ (P) \ 4a \ D_{3/2}$ $1s^{2} \ 2s^{2} \ 2s^{2} \ (P) \ 4a \ D_{3/2}$	0.00514	0.00395	C
$1s \ 2s \ 2p \ (P) \ 3p \ D_{3/2} \rightarrow 1s \ 2s \ 2p \ (P) \ 4a \ D_{5/2}$ $1s^{2} 2s^{2} 2m^{2} (^{3}\text{D}) \ 2m \ ^{4}\text{D} \qquad 1s^{2} 2s^{2} 2m^{2} (^{3}\text{D}) \ 4d \ ^{4}\text{D}$	0.00321	0.00308	C
$1s \ 2s \ 2p \ (\Gamma) \ 3p \ D_{3/2} \rightarrow 1s \ 2s \ 2p \ (\Gamma) \ 4a \ D_{3/2}$ $1s^{2} 2s^{2} 2n^{2} (^{3}\text{P}) \ 2n \ ^{4}\text{P} \rightarrow 1s^{2} 2s^{2} 2n^{2} (^{3}\text{P}) \ 4d \ ^{4}\text{P}$	0.00510	0.00030	C
$1s 2s 2p (1) 3p D_{3/2} \rightarrow 1s 2s 2p (1) 4a D_{1/2}$ $1s^2 2s^2 2n^2 (^3\mathbf{P}) 3n ^4\mathbf{D} \rightarrow 1s^2 2s^2 2n^2 (^3\mathbf{P}) 4d ^4\mathbf{D}$	0.00075	0.00780	C
$1s \ 2s \ 2p \ (\Gamma) \ 3p \ D_{5/2} \rightarrow 1s \ 2s \ 2p \ (\Gamma) \ 4a \ D_{7/2}$ $1s^{2} 2s^{2} 2n^{2} (^{3}P) \ 3n \ ^{4}D \qquad 1s^{2} 2s^{2} 2n^{2} (^{3}P) \ 4d \ ^{4}D$	0.00200	0.00223	C
$1s 2s 2p (1) 3p D_{5/2} \rightarrow 1s 2s 2p (1) 4a D_{5/2}$ $1s^2 2s^2 2n^2 (^3\mathbf{P}) 3n ^4\mathbf{D} \rightarrow 1s^2 2s^2 2n^2 (^3\mathbf{P}) 4d ^4\mathbf{D}$	0.00780	0.00897	C
$1s 2s 2p (1) 3p D_{5/2} \rightarrow 1s 2s 2p (1) 4a D_{3/2}$ $1e^2 2e^2 2n^2 (^3P) 3n ^4 D_{-4} \rightarrow 1e^2 2e^2 2n^2 (^3P) 4d ^4 D_{-4}$	0.00485	0.00347	C
$1s 2s 2p (1) 3p D_{7/2} \rightarrow 1s 2s 2p (1) 4a D_{7/2}$ $1e^2 2e^2 2n^2 (^3P) 3n ^4 D_{7/2} \rightarrow 1e^2 2e^2 2n^2 (^3P) 4d ^4 D_{7/2}$	0.0110	0.0133	C
$15 \ 25 \ 2p \ (1) \ 5p \ D_{7/2} \rightarrow 18 \ 2s \ 2p \ (1) \ 4u \ D_{5/2}$	0.00241	0.00294	C
$1s^2 2s^2 2p^2 ({}^{3}\text{P}) 3p {}^{4}\text{P}_{1/2} \rightarrow 1s^2 2s^2 2p^2 ({}^{3}\text{P}) 5d {}^{4}\text{D}_{3/2}$	0.0042	0.0044	\mathbf{C}
$1s^2 2s^2 2p^2 ({}^{3}\mathrm{P}) 3p {}^{4}\mathrm{P}_{1/2} \to 1s^2 2s^2 2p^2 ({}^{3}\mathrm{P}) 5d {}^{4}\mathrm{D}_{1/2}$	0.00830	0.00894	\mathbf{C}
$1s^2 2s^2 2p^2 ({}^{3}\mathrm{P}) 3p {}^{4}\mathrm{P}_{3/2} \to 1s^2 2s^2 2p^2 ({}^{3}\mathrm{P}) 5d {}^{4}\mathrm{D}_{5/2}$	0.00700	0.00749	\mathbf{C}
$1s^2 2s^2 2p^2 ({}^{3}\mathrm{P}) 3p {}^{4}\mathrm{P}_{3/2} \to 1s^2 2s^2 2p^2 ({}^{3}\mathrm{P}) 5d {}^{4}\mathrm{D}_{3/2}$	0.0052	0.0057	\mathbf{C}
$1s^{2}2s^{2}2p^{2}({}^{3}\mathrm{P}) 3p {}^{4}\mathrm{P}_{3/2} \to 1s^{2}2s^{2}2p^{2}({}^{3}\mathrm{P}) 5d {}^{4}\mathrm{D}_{1/2}$	0.00168	0.00178	\mathbf{C}
$1s^{2}2s^{2}2p^{2}({}^{3}\mathrm{P})3p \; {}^{4}\mathrm{P}_{5/2} \to 1s^{2}2s^{2}2p^{2}({}^{3}\mathrm{P})5d \; {}^{4}\mathrm{D}_{7/2}$	0.0099	0.0106	\mathbf{C}
$1s^{2}2s^{2}2p^{2}({}^{3}\mathrm{P})3p \; {}^{4}\mathrm{P}_{5/2} \to 1s^{2}2s^{2}2p^{2}({}^{3}\mathrm{P})5d \; {}^{4}\mathrm{D}_{5/2}$	0.00300	0.00319	\mathbf{C}
$1s^{2}2s^{2}2p^{2}\left({}^{3}\mathrm{P}\right)3p \;\; {}^{4}\mathrm{P}_{5/2} \rightarrow 1s^{2}2s^{2}2p^{2}({}^{3}\mathrm{P})5d \;\; {}^{4}\mathrm{D}_{3/2}$	0.000500	0.000531	\mathbf{C}
$1s^2 2s^2 2p^2 ({}^3\mathrm{P}) 3p^{-4}\mathrm{D}_{7/2} \rightarrow 1s^2 2s^2 2p^2 ({}^3\mathrm{P}) 5d^{-4}\mathrm{F}_{9/2}$	0.0138	0.0142	С
$1s^2 2s^2 2p^2 ({}^{3}P) 3p {}^{4}D_{5/2} \rightarrow 1s^2 2s^2 2p^2 ({}^{3}P) 5d {}^{4}F_{7/2}$	0.0126	0.0121	С
$1s^2 2s^2 2p^2 ({}^{3}P) 3p {}^{4}D_{1/2} \rightarrow 1s^2 2s^2 2p^2 ({}^{3}P) 5d {}^{4}F_{3/2}$	0.0109	0.00994	\mathbf{C}
$1s^2 2s^2 2p^2 ({}^{3}P) 3p {}^{4}D_{3/2} \rightarrow 1s^2 2s^2 2p^2 ({}^{3}P) 5d {}^{4}F_{5/2}$	0.0110	0.0106	\mathbf{C}
$1s^2 2s^2 2p^2 ({}^{3}P) 3p {}^{4}D_{3/2} \rightarrow 1s^2 2s^2 2p^2 ({}^{3}P) 5d {}^{4}F_{3/2}$	0.0043	0.0039	\mathbf{C}
$1s^2 2s^2 2p^2 ({}^{3}\text{P}) 3p {}^{4}\text{D}_{5/2} \rightarrow 1s^2 2s^2 2p^2 ({}^{3}\text{P}) 5d {}^{4}\text{F}_{5/2}$	0.00360	0.00342	\mathbf{C}
$1s^2 2s^2 2p^2 ({}^{3}\text{P}) 3p {}^{4}\text{D}_{5/2} \rightarrow 1s^2 2s^2 2p^2 ({}^{3}\text{P}) 5d {}^{4}\text{F}_{3/2}$	0.000300	0.000281	D+
$1s^2 2s^2 2p^2 ({}^{3}\text{P}) 3p {}^{4}\text{D}_{7/2} \rightarrow 1s^2 2s^2 2p^2 ({}^{3}\text{P}) 5d {}^{4}\text{F}_{7/2}$	0.00206	0.00200	\mathbf{C}
$1s^{2}2s^{2}2p^{2}(^{3}\mathrm{P}) 3p {}^{4}\mathrm{D}_{7/2} \rightarrow 1s^{2}2s^{2}2p^{2}(^{3}\mathrm{P}) 5d {}^{4}\mathrm{F}_{5/2}$	0.000143	0.000135	D+
$1s^2 2s^2 2p^2 ({}^{3}\text{P}) 3p^{-4}\text{D}_{1/2} \rightarrow 1s^2 2s^2 2p^2 ({}^{3}\text{P}) 5d^{-4}\text{D}_{1/2}$	0.00236	0.00257	С
$1s^{2}2s^{2}2p^{2}({}^{3}P) 3p {}^{4}D_{1/2} \rightarrow 1s^{2}2s^{2}2p^{2}({}^{3}P) 5d {}^{4}D_{3/2}$	0.00117	0.00129	С
$1s^{2}2s^{2}2p^{2}({}^{3}P) 3p {}^{4}D_{3/2} \rightarrow 1s^{2}2s^{2}2p^{2}({}^{3}P) 5d {}^{4}D_{3/2}$	0.00187	0.00205	\mathbf{C}
$1s^{2}2s^{2}2p^{2}({}^{3}P) 3p {}^{4}D_{3/2} \rightarrow 1s^{2}2s^{2}2p^{2}({}^{3}P) 5d {}^{4}D_{1/2}$	0.00234	0.00256	С
$1s^{2}2s^{2}2p^{2}({}^{3}P)3p {}^{4}D_{3/2} \rightarrow 1s^{2}2s^{2}2p^{2}({}^{3}P)5d {}^{4}D_{5/2}$	0.00108	0.00120	С
$1s^2 2s^2 2p^2 ({}^{3}P) 3p {}^{4}D_{5/2} \rightarrow 1s^2 2s^2 2p^2 ({}^{3}P) 5d {}^{4}D_{7/2}$	0.000650	0.000726	С
$1s^2 2s^2 2p^2 ({}^{3}P) 3p {}^{4}D_{5/2} \rightarrow 1s^2 2s^2 2p^2 ({}^{3}P) 5d {}^{4}D_{5/2}$	0.00265	0.00292	\mathbf{C}
$1s^2 2s^2 2p^2 ({}^{3}\text{P}) 3p {}^{4}\text{D}_{5/2} \rightarrow 1s^2 2s^2 2p^2 ({}^{3}\text{P}) 5d {}^{4}\text{D}_{3/2}$	0.00161	0.00178	\mathbf{C}
$1s^2 2s^2 2p^2 ({}^{3}P) 3p {}^{4}D_{7/2} \rightarrow 1s^2 2s^2 2p^2 ({}^{3}P) 5d {}^{4}D_{7/2}$	0.00388	0.00433	\mathbf{C}
$1s^2 2s^2 2p^2 ({}^3\mathrm{P}) 3p {}^4\mathrm{D}_{7/2} \to 1s^2 2s^2 2p^2 ({}^3\mathrm{P}) 5d {}^4\mathrm{D}_{5/2}$	0.000864	0.000959	\mathbf{C}
$1s^2 2s^2 2n^2 ({}^{3}\text{P}) 4n {}^{4}\text{P}_{1/2} \rightarrow 1s^2 2s^2 2n^2 ({}^{3}\text{P}) 5d {}^{4}\text{P}_{1/2}$	0.000596	0.000601	D+
$\frac{1}{1s^2 2s^2 2p^2} ({}^{3}P) 4p {}^{4}P_{2/2} \rightarrow 1s^2 2s^2 2p^2 ({}^{3}P) 5d {}^{4}P_{1/2}$	0.00294	0.00298	D+
$1s^2 2s^2 2p^2 ({}^{3}P) 4p {}^{4}P_{1/2} \rightarrow 1s^2 2s^2 2p^2 ({}^{3}P) 5d {}^{4}P_{2/2}$	0.00149	0.00148	D+
$1s^2 2s^2 2p^2 ({}^{3}P) 4p {}^{4}P_{2/2} \rightarrow 1s^2 2s^2 2p^2 ({}^{3}P) 5d {}^{4}P_{2/2}$	0.000470	0.000469	D+
$1s^2 2s^2 2p^2 ({}^{3}P) 4p {}^{4}P_{2/2} \rightarrow 1s^2 2s^2 2n^2 ({}^{3}P) 5d {}^{4}P_{7/2}$	0.00105	0.00105	D+
$1s^2 2s^2 2p^2$ (³ P) $4p^{-4} P_{5/2} \rightarrow 1s^2 2s^2 2p^2$ (³ P) $5d^{-4} P_{2/2}$	0.00153	0.00155	D+
$1s^{2}2s^{2}2p^{2} {}^{(3}P) 4p {}^{4}P_{5/2} \rightarrow 1s^{2}2s^{2}2p^{2} {}^{(3}P) 5d {}^{4}P_{5/2}$	0.00238	0.00239	D+

Table 2. Atomic transition probabilities and comparison with the accepted values taken from NIST for nitrogen.

Table 2. Continued.

Transitions	This work $(\times 10^8 \text{ sn}^{-1})$	Accepted values (Ref. [32])	Accuracy [*] (Ref. [32])
$1s^2 2s^2 2p^2 ({}^{3}\text{P}) 3p {}^{4}\text{P}_{1/2} \rightarrow 1s^2 2s^2 2p^2 ({}^{3}\text{P}) 4d {}^{4}\text{D}_{1/2}$	0.0230	0.0299	С
$1s^2 2s^2 2p^2 ({}^{3}\text{P}) 3p {}^{4}\text{P}_{1/2} \rightarrow 1s^2 2s^2 2p^2 ({}^{3}\text{P}) 4d {}^{4}\text{D}_{3/2}$	0.0115	0.0150	\mathbf{C}
$1s^2 2s^2 2p^2 ({}^{3}\text{P}) 3p {}^{4}\text{P}_{3/2} \rightarrow 1s^2 2s^2 2p^2 ({}^{3}\text{P}) 4d {}^{4}\text{D}_{5/2}$	0.0191	0.0251	\mathbf{C}
$1s^{2}2s^{2}2p^{2}({}^{3}\mathrm{P}) 3p^{-4}\mathrm{P}_{3/2} \rightarrow 1s^{2}2s^{2}2p^{2}({}^{3}\mathrm{P}) 4d^{-4}\mathrm{D}_{3/2}$	0.0146	0.0191	\mathbf{C}
$1s^2 2s^2 2p^2 ({}^{3}\text{P}) 3p {}^{4}\text{P}_{3/2} \rightarrow 1s^2 2s^2 2p^2 ({}^{3}\text{P}) 4d {}^{4}\text{D}_{1/2}$	0.00457	0.00596	\mathbf{C}
$1s^2 2s^2 2p^2 ({}^{3}\text{P}) 3p {}^{4}\text{P}_{5/2} \rightarrow 1s^2 2s^2 2p^2 ({}^{3}\text{P}) 4d {}^{4}\text{D}_{7/2}$	0.00270	0.00356	\mathbf{C}
$1s^2 2s^2 2p^2 ({}^{3}\text{P}) 3p {}^{4}\text{P}_{5/2} \rightarrow 1s^2 2s^2 2p^2 ({}^{3}\text{P}) 4d {}^{4}\text{D}_{5/2}$	0.0081	0.0107	\mathbf{C}
$1s^2 2s^2 2p^2 ({}^{3}\text{P}) 3p {}^{4}\text{P}_{5/2} \rightarrow 1s^2 2s^2 2p^2 ({}^{3}\text{P}) 4d {}^{4}\text{D}_{3/2}$	0.00135	0.00178	\mathbf{C}

* estimated accuracy rates: C $\leq 25\%$, D + $\leq 40\%.$

levels using WBEPM theory through a more simple procedure. Accuracy and reliability of the results calculated using this theory strongly depend on the accuracy and reliability of the expectation values of radius which is used in determination of Z^* , n^* and l^* parameters. The values of the transition probabilities will be better if the expectation value of radius belonging to the levels is accurate enough. We have concluded that results obtained using the expectation values of the radius calculated by nonrelativistic numerical Hartree-Fock wave functions for the relevant transitions in atomic nitrogen provides values in much better agreement with the results taken from NIST. The method used in this work requires quite shorter time than other methods need for the computation procedure. By courtesy of this method, the calculations for transition probabilities belong to either low lying or highly excited levels can easily and in a shorter time, be performed. In addition, for highly excited states, this method is also effective than other theoretical methods.

The authors gratefully acknowledge for the financial support of the Selçuk University Scientific Research Projects (BAP) Coordinating Office.

References

- E. Biemont, C.F. Fischer, M. Godefroid, N. Vaeck, A. Hibbert, Proceedings of the meeting on atomic data and oscillator strengths for Astrophysical and fusion research, edited by J.E. Hansen (North-Holland, Amsterdam, 1989) p. 59
- D.S. Leckrone, S. Johansson, R.L. Kurucz, S.J. Adelman, Proceedings of the meeting on atomic data and oscillator strengths for Astrophysical and fusion research, edited by J.E. Hansen (North-Holland, Amsterdam, 1990)
- D.R. Beck, C.A. Nicolaides, J. Quant. Spectrosc. Radiat. Transfer. 16, 297 (1976)
- 4. B.C. Fawcett, At. Data Nucl. Data Tabl. 37, 411 (1987)
- D. Hofsaess, J. Quant. Spectrosc. Radiat. Transfer 42, 45 (1989)
- M.A. Suskin, A.W. Weiss, private communication to A. Hibbert (from Ref. [8]) (1989)
- K.L. Bell, K.A. Berrington, J. Phys. At. Mol. Opt. Phys. 24, 933 (1991)

- A. Hibbert, E. Biemont, M. Godefroid, N. Vaeck, Astron. Astroph. Suppl. Ser. 88, 505 (1991)
- M. Tong, C.F. Fischer, L. Sturesson, J. Phys. B: At. Mol. Opt. Phys. 27, 4819 (1994)
- 10. C.F. Fisher, Z. Phys. D 32, 21 (1994)
- K.L. Bell, A. Hibbert, R.P. Stafford, Phys. Scripta 52, 240 (1995)
- D.J.R. Robinson, A. Hibbert, J. Phys. B: At. Mol. Opt. Phys. **30**, 4813 (1997)
- N.W. Zheng, T. Wang, R. Yang, Y.G. Wu, J. Chem. Phys. 112, 7042 (2000)
- 14. N.W. Zheng, T. Wang, Chem. Phys. 282, 31 (2002)
- 15. G.I. Tachiev, C.F. Fischer, Astron. Astrophys. 385, 716 (2002) and Vanderbilt University, Nashville, TN http://www.vuse.vanderbilt.edu/~cff/ mchf collection
- 16. N.W. Zheng, Chin. Sci. Bull. 22, 531 (1977)
- N.W. Zheng, T. Wang, T. Zhou, Y.J. Sun, Y. Su, Y. Zhang, J. Phys. Soc. Jap. 68, 3859 (1999)
- G.W. Wen, L.Y. Wang, R.D. Wang, Chin. Sci. Bull. 36, 547 (1991)
- N.W. Zheng et al., At. Data and Nucl. Data Tabl. 79, 109 (2001)
- 20. N.W. Zheng, T. Wang, Spectrochim. Acta B 58, 1319 (2003)
- 21. J. Fan, N.W. Zheng, Chem. Phys. Lett. 400, 273 (2004)
- N.W. Zheng, T. Wang, R. Yang, Y.J. Wu, J. Chem. Phys. 112, 7042 (2000)
- J. Fan, N.W. Zheng, D.X. Ma, T. Wang, Phys. Scripta 69, 398 (2004)
- 24. N.W. Zheng et al., Int. J. Quant. Chem. 76, 51 (2000)
- 25. N.W. Zheng et al., Int. J. Quant. Chem. 81, 232 (2001)
- 26. N.W. Zheng et al., Int. J. Quant. Chem. 98, 281 (2004)
- 27. C.F. Fischer, Comput. Phys. Commun. 43, 355 (1987)
- G. Gaigalas, C.F. Fischer, Comput. Phys. Commun. 98, 255 (1996)
- R.D. Cowan, The Theory of Atomic Structure and Spectra (University of California Press, Berkeley, 1981), pp. 412, 420
- Yu. Ralchenko, F.C. Jou, D.E. Kelleher, A.E. Kramida, A. Musgrove, J. Reader, W.L. Wiese, K. Olsen, *NIST Atomic Spectra Database (version 3.0.1)*, National Institute of Standards and Technology, Gaithersburg, MD (2005)
- 31. C.E. Theodosiou, Phys. Rev. A 30, 2881 (1984)
- 32. NIST Atomic Spectroscopic Database
- URL:http://physics.nist.gov Physical Reference Data (2006)