Electric-dipole allowed (E1) and forbidden (E2, M1 and M2) transition probabilities of 4f for N^{+}*

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By applying systematically enlarged multi-configuration Dirac–Fock wavefunction, the transitions for electric-dipole allowed (E1) and forbidden (E2, M1 and M2) lines are studied among 4f pair coupling and low-lying configurations for singly ionized nitrogen. Most important effects of relativity, electron correlation, the rearrangement of electron density, Breit interaction, and quantum electrodynamic effects are included in the computation. Then, allowed (E1) and forbidden (E2, M1 and M2) transition probabilities of 4f for N^{+} are obtained and compared with experimental results. Good agreement with available experimental results is found and most of the data of 4f are presented for the first time.

Keywords: allowed, forbidden, transition probability
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1. Introduction

Nitrogen is among the most abundant elements in the universe. The spectral line of 4f for NII, especially for some strong lines, mostly can be observed in astrophysics, atmospheric physics, atmospheric chemistry, laboratory plasma and other related fields.[1−5] The wavelength range for some strong lines of 4f are nearly distributed among 380–660 nm that is just the visible light range. Therefore, the investigation on the transition properties of 4f is valuable in analysing emission lines in plasma, and the transition parameters are helpful for the diagnostics of relevant plasmas.

However, So far, the theoretical work on transitions of 4f for NII is scarce, especially on transition property. Even if some theoretical methods were adopted to study the transition property of NII in the past,[6−10] but the study on 4f was not involved. 2p4f configuration has special fine structure which appears in pairs, and it can be represented by LK-coupling condition (pair coupling).[11] Since the energy level splitting is only several cm^{-1} in every pair of energy levels,[12] it is very sensitive to the influence of various effects in practical computation. Shen *et al.* have shown in detail that the influence of relativity, electron correlation, the rearrangement of electron density, Breit interaction and quantum electrodynamic effects are important in dealing with these pair configuration including fine structure and transition.[13] Thus, it brings more interest and expectation in not only studying the transition property but providing new transition parameters of this specific pair coupling configuration.

In the present work, a systematic computation on the transition among 4f and lower configurations for NII ions is carried out by adopting relativistic multi-configuration Dirac–Fock (MCDF) method. Transition probabilities of the electric-dipole allowed (E1) and forbidden (E2, M1, M2) transition among the 4f and lower configurations of NII ions are obtained, and they are in good agreement with the reported experimental results.

2. Theoretical methods and computation ways

In order to calculate energy levels and transition probabilities, wave functions have been generated by widely-used atomic structure package Grasp92 which

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is an implementation of the multi-configuration Dirac–Fock method.[14] Details on MCDF method have been presented in a number of studies.[15,16] Here, we shall restrict ourselves only to a brief account of the computational procedure.

In practical calculations, the levels are categorized concerned, according to their symmetry $J^{\rm P}$, into three groups, one for 2p4f ($J^{\rm P}$ =1^+, 2^+, 3^+, 4^+, 5^+), the second for $2p^2$, 2p3p, 2p4p ($J^{\rm P}$ = 0^+, 1^+, 2^+, 3^+), and the third for $2s^12p^3$, 2p3s, 2p3d, 2p4s, 2p4d ($J^{\rm P}$ = 0^-, 1^-, 2^-, 3^-, 4^-) (seeing Table 1). These three group configurations are chosen as reference configurations for even parity levels and odd parity levels, separately, so as to carry out a separate optimization procedure for initial and final energies and wave functions by using an extended optimal level (EOL) model of GRASP92.[13] In order to include the configuration state wave functions (CSFs) in the expansion of the wave functions as many as possible, namely to take into account the correlation effects more effectively, the active space method, which had been presented first in quantum chemistry, was used to generate the configuration state list.[14] And then, the systematically enlarged MCDF method was adopted to extend the CSFs gradually and carry out a many-step optimization until the levels and wave functions achieve a sufficient accuracy. In the computation, the electrons of $n > 1$ are considered as valence electrons. All the singe(S) and double(D) excitations from the occupied reference configurations into the unoccupied nl ($n \geq 3$, $l \leq n-1$) are included, and the correction configuration can be generated rapidly. When the correlation models are up to $6l$, nearly 20 thousand CSFs are used to obtain a sufficiently accurate description of fine structure.

Table 1. Configuration distribution in computation.

group X	upper states	lower states	$J^{\rm P}$
group 1	2p4f		$1^+ \sim 5^+$
group 2		$2p^2$	$0^+ \sim 3^+$
		2p3p	$0^+ \sim 3^+$
		2p4p	$0^+ \sim 3^+$
group 3		$2s^12p^3$	$0^- \sim 4^-$
		2p3s	$0^- \sim 4^-$
		2p3d	$0^- \sim 4^-$
		2p4s	$0^- \sim 4^-$
		2p4d	$0^- \sim 4^-$

Notation: In $J^{\rm P,P}$ stands for parity. The symbols + and − denote even parity and odd parity, respectively.

The influence of relaxation effects, namely the rearrangement of the electron density due to the emission or absorption of photons, is straightforward to be taken into consideration by the separate optimization of the initial and final states of the transition. In order to calculate the probabilities for not quite orthogonal wave functions, a developed determinant wave functions expansion program CESD99[17] and a transition probability program REOS99[18] are used. In systematically enlarged wave function expansion, the inclusion of relaxation effects typically leads to the improvement of transition probability and often requires smaller expansion to achieve a certain accuracy compared with a single orthogonal set for constructing the initial and final states together. In the present calculations, the transition probabilities are obtained from different gauges of the radiation field with Babushkin and Coulomb gauges, corresponding to the length and velocity forms, respectively. And the agreement between these two gauges can be used as a test of the quality of the wave functions.

3. Results and discussion

With the example of 4f–3d transition, Shen *et al.* have studied in detail what effects that affect 4f fine structure and transition need to be considered.[13] The results show that the influence of relativity, electron correlation and relaxation effects on 4f fine structure and transition are much more important in practical computation.[13] Breit interaction and quantum electrodynamic effects have, to some certain extent, optimized effects on energy level, even if these effects are weaker than relativity, electron correlation and relaxation effects. When the low-lying states enlarge from 3d to nearly all configurations under 4f, in order to make calculations accurate in the present work, the influence of these effects including Breit interaction and quantum electrodynamics (QED) are adequately considered in computation. Finally, the calculated wavelengths and transition probabilities of electric-dipole allowed lines among 4f and low-lying levels of NII are obtained and listed in Table 2, where transition probabilities are presented in length and velocity gauges, separately. We adopt the coupling representation with $L(K)_J$ for the reason not only the 4f states have pair coupling but also their calculation results are conveniently compared with experimental results in which 4f states are chosen to be LK coupling. In addition, W-CAL and W-OBS refer to observed wavelengths and our calculated wavelengths, respectively. Both the wavelengths and transition probabilities are compared with the available measurements.

Table 2. Wavelengths and transition probabilities of allowed lines (E1).

upper	lower	W-cal	W-obs	TP-len[a]	TP-vel[b]	TP-Exp[c]	upper	lower	W-cal	W-obs	TP-len[a]	TP-vel[b]	TP-Exp[c]
4f F(5/2)$_3$	2s^{1}2p^3 ^{3}D$^o_3$	84.91		4.90(5)	1.34(5)		4f D(5/2)$_3$	3d ^{1}D$^o_2$	419.33		4.41(6)	4.04(6)	
4f F(5/2)$_3$	2s^{1}2p^3 ^{3}D$^o_2$	85.42		1.70(6)	3.84(6)		4f D(5/2)$_3$	3d ^{3}D$^o_3$	419.79	417.9[d]	4.71(7)	4.14(7)	4.70(7)
4f F(5/2)$_3$	2s^{1}2p^3 ^{3}P$^o_2$	100.14		1.86(5)	3.73(5)		4f D(5/2)$_3$	3d ^{3}P$^o_2$	450.83	443.1[d]	1.79(8)	1.63(8)	
4f F(5/2)$_3$	2s^{1}2p^3 ^{1}D$^o_2$	157.80		6.04(6)	1.00(7)		4f D(5/2)$_3$	3d ^{1}F$^o_3$	456.13		8.66(5)	9.01(5)	
4f F(5/2)$_3$	3d ^{3}F$^o_3$	412.69		1.31(7)	1.06(7)		4f D(5/2)$_3$	4s ^{3}P$^o_2$	681.21		9.05(5)	7.86(5)	
4f F(5/2)$_3$	3d ^{1}D$^o_2$	426.26	417.62[e]	1.28(8)	1.17(8)	1.13(8)	4f D(5/2)$_2$	2s^{1}2p^3 ^{3}D$^o_3$	84.64		4.30(5)	1.37(5)	
4f F(5/2)$_3$	3d ^{3}D$^o_2$	431.87		7.28(7)	6.66(7)		4f D(5/2)$_2$	2s^{1}2p^3 ^{3}D$^o_2$	85.15		3.16(5)	8.68(5)	
4f F(5/2)$_3$	3d ^{3}D$^o_3$	426.74		4.06(6)	3.24(6)		4f D(5/2)$_2$	2s^{1}2p^3 ^{3}P$^o_2$	99.77		3.99(5)	8.33(5)	
4f F(5/2)$_3$	3d ^{3}P$^o_2$	458.85		7.74(6)	7.10(6)		4f D(5/2)$_2$	2s^{1}2p^3 ^{3}P$^o_1$	98.88		1.93(6)	2.27(6)	
4f F(5/2)$_3$	3d ^{1}F$^o_3$	464.35		1.08(7)	1.08(7)		4f D(5/2)$_2$	2s^{1}2p^3 ^{1}D$^o_2$	156.88		8.25(5)	1.58(6)	
4f F(5/2)$_2$	2s^{1}2p^3 ^{3}D$^o_2$	85.41		4.82(5)	1.11(6)		4f D(5/2)$_2$	3s ^{3}P$^o_1$	159.95		1.64(5)	3.70(5)	
4f F(5/2)$_2$	2s^{1}2p^3 ^{3}D$^o_1$	84.84		5.47(6)	6.66(6)		4f D(5/2)$_2$	3s ^{3}P$^o_2$	161.03		3.62(4)	1.50(5)	
4f F(5/2)$_2$	2s^{1}2p^3 ^{1}P$^o_1$	237.64		1.72(5)	1.98(5)		4f D(5/2)$_2$	2s^{1}2p^3 ^{1}P$^o_1$	235.59		3.30(6)	3.84(6)	
4f F(5/2)$_2$	3d ^{3}F$^o_2$	416.15		2.12(7)	2.07(7)	0.80(7)	4f D(5/2)$_2$	3d ^{3}F$^o_3$	406.47		1.19(6)	5.18(5)	
4f F(5/2)$_2$	3d ^{3}F$^o_3$	412.61		2.54(6)	2.46(6)		4f D(5/2)$_2$	3d ^{1}D$^o_2$	419.63	410.8[d]	1.18(7)	1.20(7)	
4f F(5/2)$_2$	3d ^{1}D$^o_2$	426.18	417.5[d]	1.44(6)	1.44(6)		4f D(5/2)$_2$	3d ^{3}D$^o_2$	425.06		2.45(7)	2.39(7)	1.20(7)
4f F(5/2)$_2$	3d ^{3}D$^o_1$	426.16	423.5[d]	1.85(8)	1.73(8)		4f D(5/2)$_2$	3d ^{3}D$^o_3$	420.09		4.51(6)	4.07(6)	
4f F(5/2)$_2$	3d ^{3}D$^o_2$	431.79		2.85(7)	2.64(7)		4f D(5/2)$_2$	3d ^{3}P$^o_2$	451.18		2.77(7)	2.60(7)	
4f F(5/2)$_2$	3d ^{3}D$^o_3$	426.66		7.30(5)	6.57(5)		4f D(5/2)$_2$	3d ^{3}P$^o_1$	446.16	444.0[d]	8.24(7)	7.71(7)	6.95(7)
4f F(5/2)$_2$	3d ^{3}P$^o_2$	458.76		1.19(5)	1.14(5)		4f D(5/2)$_2$	3d ^{1}F$^o_3$	456.49		8.00(5)	1.84(5)	
4f F(5/2)$_2$	3d ^{3}P$^o_1$	453.57		4.75(5)	4.44(5)		4f D(5/2)$_2$	3d ^{1}P$^o_1$	472.26	469.4[d]	7.53(7)	6.94(7)	6.07(7)
4f F(5/2)$_2$	3d ^{1}P$^o_1$	480.58		2.68(6)	2.39(6)		4f D(5/2)$_2$	4s ^{3}P$^o_1$	666.93		2.62(5)	2.52(5)	
4f F(7/2)$_3$	2s^{1}2p^3 ^{3}D$^o_3$	84.88		9.97(5)	3.59(5)		4f D(5/2)$_2$	4s ^{3}P$^o_2$	682.02		1.29(5)	1.20(5)	
4f F(7/2)$_3$	2s^{1}2p^3 ^{3}D$^o_2$	85.40		1.51(6)	3.42(6)		4f D(5/2)$_2$	4s ^{1}P$^o_1$	731.10		8.54(5)	8.63(5)	
4f F(7/2)$_3$	2s^{1}2p^3 ^{1}D$^o_2$	157.73		5.03(6)	8.48(6)		4f D(3/2)$_1$	2s^{1}2p^3 ^{3}D$^o_2$	85.08		1.29(5)	3.72(5)	
4f F(7/2)$_3$	3d ^{3}F$^o_2$	415.74	407.2[d]	6.31(7)	5.90(7)	4.99(7)	4f D(3/2)$_1$	2s^{1}2p^3 ^{3}D$^o_1$	84.51		5.79(5)	7.77(5)	
4f F(7/2)$_3$	3d ^{3}F$^o_3$	412.21		1.06(6)	1.30(6)		4f D(3/2)$_1$	2s^{1}2p^3 ^{3}P$^o_2$	99.68		5.72(4)	1.28(5)	
4f F(7/2)$_3$	3d ^{1}D$^o_2$	425.76	417.0[d]	5.44(7)	4.93(7)	4.48(7)	4f D(3/2)$_1$	2s^{1}2p^3 ^{3}P$^o_1$	98.80		1.67(6)	1.98(6)	
4f F(7/2)$_3$	3d ^{3}D$^o_2$	431.34		9.86(7)	8.90(7)		4f D(3/2)$_1$	2s^{1}2p^3 ^{3}P$^o_0$	98.84		1.20(6)	2.93(6)	
4f F(7/2)$_3$	3d ^{3}D$^o_3$	426.23		1.13(7)	9.78(6)		4f D(3/2)$_1$	3s ^{3}P$^o_0$	159.23		1.53(5)	5.88(5)	
4f F(7/2)$_3$	3d ^{1}F$^o_3$	463.74		9.51(6)	8.94(6)		4f D(3/2)$_1$	3s ^{3}P$^o_1$	159.72		1.21(5)	4.23(5)	
4f F(7/2)$_4$	2s^{1}2p^3 ^{3}D$^o_3$	84.88		2.39(7)	3.87(6)		4f D(3/2)$_1$	3d ^{3}F$^o_2$	408.43		1.33(6)	3.00(5)	
4f F(7/2)$_4$	3d ^{3}F$^o_3$	412.07	408.1[d]	4.85(7)	4.01(7)	3.35(7)	4f D(3/2)$_1$	3d ^{3}D$^o_1$	418.07		2.52(7)	2.40(7)	
4f F(7/2)$_4$	3d ^{3}F$^o_4$	409.24		1.44(7)	1.42(7)		4f D(3/2)$_1$	3d ^{3}D$^o_2$	423.48		8.81(6)	8.07(6)	
4f F(7/2)$_4$	3d ^{3}D$^o_3$	426.08	424.1[d]	1.96(8)	1.76(8)		4f D(3/2)$_1$	3d ^{3}P$^o_2$	449.40		5.93(6)	5.33(6)	
4f F(7/2)$_4$	3d ^{1}F$^o_3$	463.57		8.81(6)	9.03(6)		4f D(3/2)$_1$	3d ^{3}P$^o_1$	444.42		8.27(7)	7.46(7)	
4f G(7/2)$_3$	2s^{1}2p^3 ^{3}D$^o_2$	85.23		2.31(5)	5.27(5)		4f D(3/2)$_1$	3d ^{3}P$^o_0$	453.64		1.30(8)	8.98(7)	
4f G(7/2)$_3$	2s^{1}2p^3 ^{1}D$^o_2$	157.15		1.06(6)	1.77(6)		4f D(3/2)$_1$	4s ^{3}P$^o_1$	663.05		4.08(5)	3.32(5)	
4f G(7/2)$_3$	3d ^{3}F$^o_2$	411.75	403.4[d]	1.65(8)	1.54(8)	1.30(8)	4f D(3/2)$_1$	4s ^{3}P$^o_0$	681.16		1.08(6)	7.39(5)	
4f G(7/2)$_3$	3d ^{3}F$^o_3$	408.29	404.4[d]	2.90(7)	2.58(7)	2.14(7)	4f D(3/2)$_2$	2s^{1}2p^3 ^{3}D$^o_3$	84.57		3.34(5)	8.19(4)	
4f G(7/2)$_3$	3d ^{1}D$^o_2$	421.57	413.1[d]	2.24(7)	2.05(7)	2.04(7)	4f D(3/2)$_2$	2s^{1}2p^3 ^{3}D$^o_2$	85.07		1.13(5)	3.59(5)	
4f G(7/2)$_3$	3d ^{3}D$^o_2$	427.05		2.38(7)	2.14(7)		4f D(3/2)$_2$	2s^{1}2p^3 ^{3}D$^o_1$	84.50		8.11(4)	1.56(5)	
4f G(7/2)$_3$	3d ^{3}D$^o_3$	422.04		2.68(6)	2.41(6)		4f D(3/2)$_2$	2s^{1}2p^3 ^{3}P$^o_2$	99.67		2.67(5)	6.20(5)	
4f G(7/2)$_3$	3d ^{1}F$^o_3$	458.78		2.62(6)	2.20(6)		4f D(3/2)$_2$	2s^{1}2p^3 ^{3}P$^o_1$	98.78		1.27(6)	1.73(6)	
4f G(7/2)$_3$	4d ^{3}F$^o_2$	6420.9		1.26(5)	7.38(4)		4f D(3/2)$_2$	2s^{1}2p^3 ^{1}D$^o_2$	156.63		9.84(5)	1.92(6)	
4f G(7/2)$_4$	2s^{1}2p^3 ^{3}D$^o_3$	84.72		2.91(6)	5.82(5)		4f D(3/2)$_2$	3s ^{3}P$^o_1$	159.69		7.36(4)	3.15(5)	
4f G(7/2)$_4$	3d ^{3}F$^o_3$	408.40	404.35[e]	1.30(8)	1.13(8)	1.25(8)	4f D(3/2)$_2$	3s ^{3}P$^o_2$	160.76		2.88(4)	1.19(5)	
4f G(7/2)$_4$	3d ^{3}F$^o_4$	405.61	405.6[d]	2.54(7)	2.41(7)	1.99(7)	4f D(3/2)$_2$	2s^{1}2p^3 ^{1}P$^o_1$	235.02		3.98(6)	4.73(6)	
4f G(7/2)$_4$	3d ^{3}D$^o_3$	422.16	419.8[d]	3.63(7)	3.25(7)		4f D(3/2)$_2$	3d ^{3}F$^o_3$	404.79		5.40(5)	1.23(5)	
4f G(7/2)$_4$	3d ^{1}F$^o_3$	458.93	455.2[d]	6.50(7)	6.88(7)	6.11(7)	4f D(3/2)$_2$	3d ^{1}D$^o_2$	417.84	409.6[d]	2.21(7)	2.22(7)	
4f G(9/2)$_5$	3d ^{3}F$^o_4$	404.27	404.1[d]	2.78(8)	2.56(8)	2.08(8)	4f D(3/2)$_2$	3d ^{3}D$^o_1$	417.82		4.90(6)	4.82(6)	
4f G(9/2)$_4$	2s^{1}2p^3 ^{3}D$^o_3$	84.65		1.03(6)	1.26(3)		4f D(3/2)$_2$	3d ^{3}D$^o_2$	423.22		5.14(6)	5.08(6)	
4f G(9/2)$_4$	3d ^{3}F$^o_3$	406.67	402.5[d]	7.94(7)	7.96(7)	6.72(7)	4f D(3/2)$_2$	3d ^{3}D$^o_3$	418.30		2.72(6)	2.44(6)	
4f G(9/2)$_4$	3d ^{3}F$^o_4$	403.91		5.95(6)	5.27(6)		4f D(3/2)$_2$	3d ^{3}P$^o_2$	449.11	441.7[d]	2.33(7)	2.18(7)	2.33(7)
4f G(9/2)$_4$	3d ^{3}D$^o_3$	420.31		1.96(5)	3.50(5)		4f D(3/2)$_2$	3d ^{3}P$^o_1$	444.13	442.5[d]	6.06(7)	5.72(7)	5.68(7)
4f G(9/2)$_4$	3d ^{1}F$^o_3$	456.75	452.9[d]	1.49(8)	1.44(8)	1.45(8)	4f D(3/2)$_2$	3d ^{1}F$^o_3$	454.37		1.03(6)	3.12(5)	
4f D(5/2)$_3$	2s^{1}2p^3 ^{3}D$^o_3$	84.63		5.87(6)	1.43(6)		4f D(3/2)$_2$	3d ^{1}P$^o_1$	470.00	467.7[d]	1.03(8)	9.56(7)	
4f D(5/2)$_3$	2s^{1}2p^3 ^{3}P$^o_2$	99.75		2.62(6)	5.25(6)		4f D(3/2)$_2$	4s ^{3}P$^o_1$	662.42		3.32(5)	3.24(5)	
4f D(5/2)$_3$	2s^{1}2p^3 ^{1}D$^o_2$	156.84		3.50(5)	5.69(5)		4f D(3/2)$_2$	4s ^{3}P$^o_2$	677.30		1.04(5)	9.55(4)	
4f D(5/2)$_3$	3s ^{3}P$^o_2$	160.98		2.92(5)	1.05(6)		4f D(3/2)$_2$	4s ^{1}P$^o_1$	725.68		9.47(5)	9.70(5)	
4f D(5/2)$_3$	3d ^{3}F$^o_3$	406.18		1.89(4)	1.20(5)								

Notation:[a]Transition probabilities of length gauge in this work. [b] Transition probabilities of velocity gauge in this work. [c]Experimental transition probabilities cited from Ref.[19]. [d]Date cited from Ref.[20]. [e]Date cited from Ref. [19].

The transition of 4f–3d is the main radiation from 4f, that is why 4f–3d transition has been chosen to study how many important effects the pair coupling configuration can offer. It is clear from Table 2 that most allowed transition probabilities with $10^7 s^{-1}$ and 10^8 s^{-1} belong to 4f–3d and are in good agreement with experimental data.[19] Except Mar′*s* results, there are few experimental transition probabilities of 4f–3d available that can be used for comparing the present results. 4f $G(9/2)_5$–3d $^3F^o_4$ with the wavelength of 404.1 nm has the maximum transition probability which is up to 2.78×10^8 s^{-1}. In spectroscopic observation involving 4f transition lines, even in the visible ray range, 404.1 nm appeared determinately.[1−5] Apart from this line, there is another strong line with a wavelength of 424.18 nm which is not referred by Mar *et al.*[19] This line is similar to 404.1 nm and has been observed obviously in many experiments.[1,20−22] In the present work, the calculated transition probability of this line is 10^8 s^{-1}. In addition, the agreement between length and velocity gauge is good for the transition probabilities larger than 10^7 s^{-1}.

Wavelengths and transition probabilities of 4f–$2s^12p^3$, 3s, 4s, 4d are also calculated, and the results are listed in Table 2, where the transition probabilities under 10^5 s^{-1} are not given. It can be seen from the results that most of these transition probabilities are lower than 10^7 s^{-1}. Though there are no reported experimental data to compare with our results, most values in length and velocity gauge are in accordance with the measurements in order of magnitude. Apart from 4f–3d, 4f–$2s^12p^3$ is the main radiative transition, 4f–3s follows back, and 4f–4s is weaker transition than 4f–3s. In all allowed lines for 4f spectrum, 4f–4d is the weakest transition. Most transition probabilities of 4f–4d are 3 orders of magnitude less than those of 4f–3d. The maximum transition of 4f–4d is $G(7/2)_3$–$^3F^o_2$ with a probability of 1.26×10^5 s^{-1}.

Table 3. Transition probabilities of forbidden lines (E2, M1 and M2).

Trans.	multiplet	$J^P - J^P$	type	TP-len	TP-vel	TP-m[a]	Trans.	multiplet	J^P-J^P	type	TP-len	TP-vel	TP-m[a]
4f-3p	F(7/2)-^{3}D	4^+-3^+	E2	4.35(+2)	3.48(+2)		4f-$2p^2$	D(3/2)-^{1}D	2^+-2^+	E2	1.14(+3)	3.53(+2)	
4f-3p	G(7/2)-^{3}D	4^+-3^+	E2	7.60(+2)	6.02(+2)		4f-$2p^2$	D(3/2)-^{1}D	2^+-2^+	M1			1.23
4f-3p	G(9/2)-^{3}D	4^+-3^+	E2	1.76(+2)	1.38(+2)		4f-3p	D(3/2)-^{3}D	2^+-2^+	M1			2.45
4f-3p	F(5/2)-^{3}D	3^+-3^+	M1			4.92(-1)	4f-3p	D(3/2)-^{3}P	2^+-2^+	E2	2.46(+2)	2.52(+2)	
4f-3p	G(7/2)-^{3}D	3^+-3^+	E2	1.15(+2)	9.14(+1)		4f-3p	D(3/2)-^{3}P	2^+-2^+	M1			2.59(-2)
4f-3p	D(5/2)-^{3}D	3^+-3^+	E2	2.39(+2)	1.78(+2)		4f-3p	D(3/2)-^{1}D	2^+-2^+	M1			1.64
4f-3p	D(5/2)-^{3}D	3^+-3^+	M1			7.13	4f-$2p^2$	F(5/2)-^{3}P	2^+-1^+	E2	7.83(+3)	2.61(+3)	
4f-4p	D(5/2)-^{3}D	3^+-3^+	M1			2.98(-3)	4f-3p	F(5/2)-^{3}D	2^+-1^+	E2	5.46(+2)	4.73(+2)	
4f-$2p^2$	F(5/2)-^{3}P	3^+-2^+	E2	5.44(+2)	3.16(+2)		4f-3p	F(5/2)-^{3}D	2^+-1^+	M1			4.72(-3)
4f-$2p^2$	F(5/2)-^{1}D	3^+-2^+	E2	4.14(+3)	1.63(+3)		4f-3p	F(5/2)-^{3}P	2^+-1^+	E2	4.93(+2)	5.49(+2)	
4f-3p	F(5/2)-^{3}D	3^+-2^+	E2	3.18(+2)	2.88(+2)		4f-$2p^2$	D(5/2)-^{3}P	2^+-1^+	E2	1.19(+3)	4.88(+2)	
4f-3p	F(5/2)-^{3}D	3^+-2^+	M1			2.72(-2)	4f-3p	D(5/2)-^{1}P	2^+-1^+	E2	7.35(+2)	5.81(+2)	
4f-3p	F(5/2)-^{1}D	3^+-2^+	E2	2.08(+2)	2.18(+2)		4f-3p	D(5/2)-^{3}D	2^+-1^+	M1			3.32(-1)
4f-$2p^2$	F(7/2)-^{3}P	3^+-2^+	E2	8.96(+2)	8.57(+2)		4f-3p	D(5/2)-^{3}S	2^+-1^+	E2	5.80(+2)	5.53(+2)	
4f-$2p^2$	F(7/2)-^{1}D	3^+-2^+	E2	1.56(+3)	1.28(+3)		4f-3p	D(5/2)-^{3}P	2^+-1^+	E2	1.14(+2)	1.28(+2)	
4f-3p	F(7/2)-^{3}P	3^+-2^+	E2	1.14(+2)	1.71(+2)		4f-$2p^2$	D(3/2)-^{3}P	2^+-1^+	E2	2.74(+2)	9.34(+1)	
4f-3p	F(7/2)-^{1}D	3^+-2^+	E2	1.24(+2)	2.37(+2)		4f-3p	D(3/2)-^{1}P	2^+-1^+	E2	9.11(+2)	7.01(+2)	
4f-$2p^2$	G(7/2)-^{1}D	3^+-2^+	E2	2.16(+1)	2.60(+2)		4f-3p	D(3/2)-^{3}D	2^+-1^+	M1			2.47(-1)
4f-3p	G(7/2)-^{3}D	3^+-2^+	E2	5.21(+2)	7.02(+2)		4f-3p	D(3/2)-^{3}S	2^+-1^+	E2	5.03(+2)	4.70(+2)	
4f-$2p^2$	D(5/2)-^{3}P	3^+-2^+	E2	6.53(+3)	3.40(+3)		4f-$2p^2$	D(3/2)-^{3}P	1^+-2^+	E2	1.24(+3)	8.65(+2)	
4f-$2p^2$	D(5/2)-^{1}D	3^+-2^+	E2	4.96(+2)	1.06(+2)		4f-$2p^2$	D(3/2)-^{1}D	1^+-2^+	E2	1.55(+2)	1.31(+0)	
4f-3p	D(5/2)-^{3}D	3^+-2^+	M1			3.88(-1)	4f-$2p^2$	D(3/2)-^{1}D	1^+-2^+	M1			1.42(-3)
4f-3p	D(5/2)-^{3}P	3^+-2^+	E2	7.96(+2)	8.34(+2)		4f-3p	D(3/2)-^{3}D	1^+-2^+	M1			1.02
4f-3p	D(5/2)-^{3}P	3^+-2^+	M1			1.24(-3)	4f-3p	D(3/2)-^{3}P	1^+-2^+	E2	2.10(+2)	2.62(+2)	
4f-3p	D(5/2)-^{3}D	2^+-3^+	M1			1.89(-1)	4f-3p	D(3/2)-^{3}P	1^+-2^+	M1			6.57(-3)
4f-3p	D(3/2)-^{3}D	2^+-3^+	M1			1.36(-1)	4f-3p	D(3/2)-^{1}D	1^+-2^+	M1			2.38(-3)
4f-$2p^2$	F(5/2)-^{3}P	2^+-2^+	E2	1.82(+2)	2.40(+2)		4f-$2p^2$	D(3/2)-^{3}P	1^+-1^+	E2	8.08(+3)	2.65(+3)	
4f-$2p^2$	F(5/2)-^{1}D	2^+-2^+	E2	3.27(+2)	1.92(+1)		4f-3p	D(3/2)-^{1}P	1^+-1^+	M1			1.81(-3)
4f-$2p^2$	F(5/2)-^{1}D	2^+-2^+	M1			6.51(-2)	4f-3p	D(3/2)-^{3}D	1^+-1^+	M1			3.54(-1)
4f-3p	F(5/2)-^{3}D	2^+-2^+	E2	2.36(+2)	2.98(+2)		4f-3p	D(3/2)-^{3}S	1^+-1^+	E2	1.05(+3)	9.83(+2)	
4f-3p	F(5/2)-^{3}D	2^+-2^+	M1			3.33(-2)	4f-3p	D(3/2)-^{3}P	1^+-1^+	E2	6.58(+2)	7.43(+2)	
4f-3p	F(5/2)-^{1}D	2^+-2^+	M1			7.90(-2)	4f-3p	D(3/2)-^{3}P	1^+-1^+	M1			2.61(-3)
4f-$2p^2$	D(5/2)-^{3}P	2^+-2^+	E2	2.04(+3)	1.53(+3)		4f-3d	G(9/2)-^{3}F^o	5^+-4^-	M2			3.10(-3)
4f-$2p^2$	D(5/2)-^{1}D	2^+-2^+	E2	1.21(+2)	2.53(+2)		4f-$2s^12p^3$	F(7/2)-^{3}D^o	4^+-3^-	M2			4.97(-3)
4f-$2p^2$	D(5/2)-^{1}D	2^+-2^+	M1			1.15	4f-3d	F(7/2)-^{3}D^o	4^+-3^-	M2			1.72(-3)
4f-3p	D(5/2)-^{3}D	2^+-2^+	M1			2.62	4f-3d	G(7/2)-^{3}F^o	4^+-3^-	M2			1.47(-3)
4f-3p	D(5/2)-^{3}P	2^+-2^+	E2	2.89(+2)	3.74(+2)		4f-$2s^12p^3$	D(5/2)-^{3}D^o	3^+-3^-	M2			2.98(-3)
4f-3p	D(5/2)-^{3}P	2^+-2^+	M1			1.21(-3)	4f-3d	D(5/2)-^{3}D^o	3^+-3^-	M2			1.03(-3)
4f-3p	D(5/2)-^{1}D	2^+-2^+	M1			1.63	4f-3d	D(5/2)-^{3}P^o	3^+-2^-	M2			1.28(-3)
4f-$2p^2$	D(3/2)-^{3}P	2^+-2^+	E2	1.79(+3)	8.96(+2)								

Notation: [a]Magnetic transition probabilities in this work.

The forbidden transition, i.e. electric quadrupole radiation (E2), magnetic dipole radiation (M1) and magnetic quadrupole radiation (M2) among 4f and low-lying configuration are also calculated and presented in Table 3. In the present data listed, we give only the transition probabilities of E2 transition larger than 10^2 s^{-1} and those of M1, M2 transition larger than 10^{-3} s^{-1}. It is shown that the maximal value is about 10^3 s^{-1}. The orders of magnitude for E2 transition probabilities in length and in velocity gauge are mostly similar to each other.

4. Conclusions

By applying the relativistic multi-configuration Dirac–Fock method, wavelength and transition probabilities for electric-dipole allowed (E1) and forbidden (E2, M1 and M2) transitions among 4f and low-lying configurations for NII are calculated by considering the most important effects of relativity, electron correlation, the rearrangement of the electron density, Breit interaction and quantum electrodynamic effects. And then, allowed (E1) and forbidden (E2, M1 and M2) transition probabilities of 4f are obtained. The results are in satisfactory agreement with experiment values, and these new 4f transition parameters will be helpful for the future plasma study.

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References

[1] Dempsey J T, Storey J W V and Phillips A 2005 *Proc. Astron. Soc. Aust.* **22** 91
[2] Mark Robertson-Tessi and Donald R Garnett 2005 *Astrophys. J. Suppl. S.* **157** 371
[3] Vladimir Escalante and Christophe Morisset 2005 *Mon. Not. R. Astron. Soc.* **361** 813
[4] Liu X W, Barlow M J, Zhang Y, Bastin R J and Storey P J 2006 *Mon. Not. R. Astron. Soc.* **368** 1959
[5] Morel T, Butler K, Aerts C, Neiner C and Briquet M 2006 *Astron. Astrophys.* **457** 651
[6] Luo D and Pradhan A K 1989 *J. Phys.* B: *At. Mol. Opt. Phys.* **22** 3377
[7] Bell K L, Ramsbottom C A and Hibbert A 1992 *J. Phys.* B: *At. Mol. Opt. Phys.* **25** 1735
[8] Bell K L, Hibbert A and Stafford R P 1995 *Phys. Scr.* **52** 240
[9] Lavin C, Olalla E and Martin I 2000 *Astrophys. J.* **543** 1051
[10] Yuan P, Liu X S, Zhang Y J, Xie L Y and Dong C Z 2002 *Acta. Phys. Sin.* **51** 2495 (in Chinese)
[11] Cowan R D 1981 *The Theory of Atomic Structure and Spectra* (London: University of California Press) p128
[12] Moore C E 1971 *Atomic Energy Levels, Natl. Stand. Ref. Data Ser., Natl. Bur. Stand.* 35 Vol. I.(U. S.)
[13] Shen X Z, Yuan P, Li J G, Dong C Z, Xie L Y and Shi Y L 2007 *Acta Phys. Sin.* **56** 5715 (in Chinese)
[14] Parpia F A, Fischer C F and Grant I P 1996 *Comput. Phys. Commun.* **94** 249
[15] Grant I P In: 1988 *Methods in Computational Chemistry* Vol.2 (New York: Plenum Press)
[16] Dong C Z and Fritzsche S 2005 *Phys. Rev.* A **72** 012507
[17] Fritzsche S and Anton J 2000 *Comput. Phys. Commun.* **124** 353
[18] Fritzsche S, Froese Fischer C and Dong C Z 2000 *Comput. Phys. Commun.* **124** 340
[19] Mar S, Perez C, Gonzalez V R, Gigosos M A, del Val1 J A, de la Rosa I and Aparicio J A 2000 *Astron. Astrophys. Suppl. Ser.* **144** 509
[20] Marquette A, Gisselbrecht M, Benten W and Meyer M 2000 *Phys. Rev.* A **62** 022513
[21] Baldwin J A, Verner E M, Verner D A, Ferland G J, Martin P G, Korista K T and Rubin R H 2000 *Astrophys. J. Suppl. S.* **129** 229
[22] Liu X W, Luo S G, Barlow M J, Danziger I J and Storey P J 2001 *Mon. Not. R. Astron. Soc.* **327** 141