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ARTICLE

Theoretical Calculation on Isotope Shifts of N(I)

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The special mass shift coefficient and field parameter factor of four multiples, $3s^4P \rightarrow 3p^4P^\circ$, $3s^4P \rightarrow 3p^4D^\circ$, $3s^2D \rightarrow 5p^2D^\circ$, and $3s^2P \rightarrow 3p^2P^\circ$, of ^{14}N and ^{15}N were studied using the multi-configuration Dirac-Hartree-Fock method and the relativistic configuration interaction approach. The normal mass shifts, special mass shifts, field shifts, and isotope shifts of N(I) were derived from the theoretical calculated normal mass shift parameter, special mass shift parameter and field parameter factor, and compared with the reported experimental measurements and theoretical results.

Key words: Multi-configuration Dirac-Hartree-Fock, Relativistic configuration interaction, Isotope shifts, Specific mass shifts

I. INTRODUCTION

Studying isotope shifts (ISs) is one of the effective methods to investigate the properties of atomic nucleus. Information, such as, nuclear charge distribution, nuclear spin, and hyperfine structure can be obtained by studying the ISs of atoms. In the field of fundamental physics, ISs can be used to test quantum mechanical calculation method and standard model theory, and study the spatial-temporal evolution properties of the fine structure constant α [1–3]. In astrophysics area, ISs can be used to study the nature of black hole and Hawking radiation [4, 5]. In recent years, the isotope shift method has attracted a great deal of interest, and been widely applied to precision measurement of unstable nucleus and estimation of the nuclear root mean square (RMS) charge radii $\delta\langle r^2 \rangle$ [6, 7]. ISs also can be used in precision measurement of atomic and molecular spectrum, optical frequency standard, cold atomic physics, atomic laser cooling and trapping [8–10]. As one of the richest elements on the earth, nitrogen atom has important applications in the fields of physical chemistry, combustion kinetics, plasma physics and astrophysics [11–13].

Holmes [14, 15] studied isotope shifts of $3s^4P_{J''} \rightarrow 3p^4P_{J'}^\circ$, $3s^2P_{J''} \rightarrow 3p^2P_{J'}^\circ$, and $3s^4P_{J''} \rightarrow 3p^4D_{J'}^\circ$ transitions of ^{14}N - ^{15}N isotopic pair by fitting the measurement data to a second-order interpolation formula. Cangiano *et al.* [16] reported isotope shifts of $3s^4P_{J''} \rightarrow 3p^4P_{J'}^\circ$ using external cavity diode laser and Doppler-free technique. Jennerich *et al.* [17] measured isotope shifts of $3s^4P_{J''} \rightarrow 3p^4P_{J'}^\circ$, and $3s^4P_{J''} \rightarrow 3p^4D_{J'}^\circ$ transitions using saturated absorption

spectroscopy method. In our previous experiment, we studied ISs of $3s^4P_{J''} \rightarrow 3p^4P_{J'}^\circ$, $3s^4P_{J''} \rightarrow 3p^4D_{J'}^\circ$, $3s^2D_{J''} \rightarrow 5p^2D_{J'}^\circ$, and $3p^2P_{J''} \rightarrow 5s^2P_{J'}^\circ$ transitions by measuring the Doppler-limited absorption spectra of ^{14}N and ^{15}N atoms using concentration modulation spectroscopy [18].

However, the theoretical investigation of the ISs of N(I) is scarce. Carette *et al.* [19] gave the specific mass shifts of $3s^4P_{J''} \rightarrow 3p^4D_{J'}^\circ$ and $3s^4P_{J''} \rightarrow 3p^4P_{J'}^\circ$ based on Jennerich's experimental results [17] and Jöhsson's *ab initio* values [20]. In the present work, special mass shift parameters, field factors, and the isotope shifts of the $3s^4P \rightarrow 3p^4P^\circ$, $3s^4P \rightarrow 3p^4D^\circ$, $3s^2D \rightarrow 5p^2D^\circ$, and $3s^2P \rightarrow 3p^2P^\circ$ transitions were calculated and compared with the reported experimental and theoretical results. The schematic energy level diagram of the four transitions is shown in FIG. 1.

II. THEORETICAL METHODS

The isotope shift is made up of two parts: the field shift (FS) and the mass shift (MS). The MS usually consists of two parts: the normal mass shift (NMS) and the specific mass shift (SMS). Spectral transition frequency ν_{ul} from the upper energy level E_u to the lower energy level E_l can be expressed as:

$$\nu_{ul} = \frac{E_u - E_l}{h} \quad (1)$$

The isotope shift $\delta\nu^{M,M'}$ can be expressed as [22]:

$$\Delta\nu^{M,M'} = (\Delta K^{\text{NMS}} + \Delta K^{\text{SMS}}) \left(\frac{1}{M} - \frac{1}{M'} \right) + F_{ul} \delta\langle r^2 \rangle^{M,M'} \quad (2)$$

where ΔK^{NMS} and ΔK^{SMS} are the normal mass shift parameter and the special mass shift parameter, respectively. F_{ul} is the field parameter factor, M and M' are

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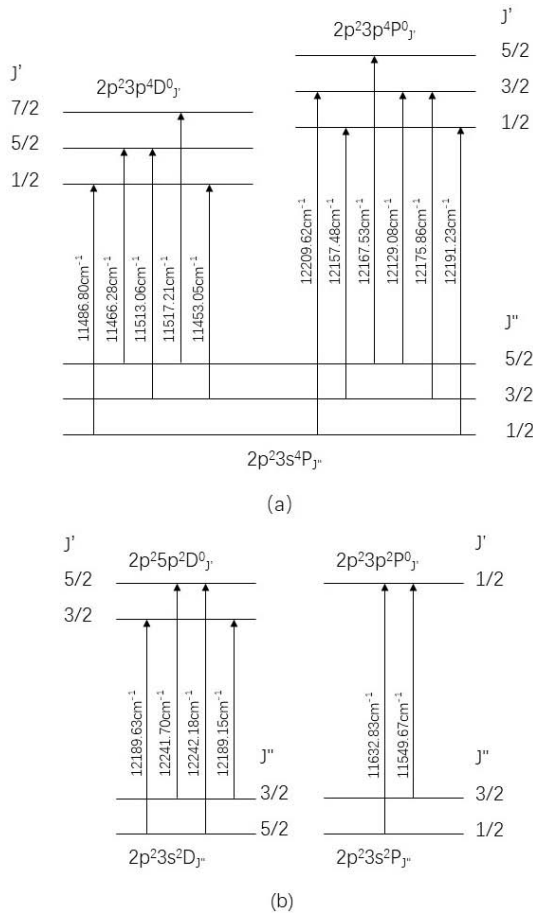


FIG. 1 (a) Schematic energy level diagram of the $2p^23s^4P_{J''}$, $2p^23p^4D_{J'}$, and $2p^23p^4P_{J'}$ states. (b) Schematic energy level diagram of the $2p^23s^2D_{J''}$, $2p^25p^2D_{J'}$, $2p^23s^2P_{J''}$, and $2p^23p^2P_{J'}$ states. The transition frequencies are from NIST database [21].

the nuclear mass of isotopes. $\delta\langle r^2 \rangle^{M,M'}$ is the difference of the nuclear rms charge radii of isotopes.

$$\Delta K^{\text{SMS}} = K_u^{\text{SMS}} - K_l^{\text{SMS}}$$

$$K_i^{\text{SMS}} = M \langle \Psi_i | H_{\text{SMS}} | \Psi_i \rangle$$

The special mass shift operator, H_{SMS} , can be expressed as [23]:

$$H_{\text{SMS}} = \frac{1}{2M} \sum_{i \neq j} \left\{ \vec{p}_i \vec{p}_j - \frac{\alpha Z}{r_i} \left[\vec{\alpha}_i + \frac{(\vec{\alpha}_i \cdot \vec{r}_i) \vec{r}_i}{r_i^2} \right] \cdot \vec{p}_j \right\} \quad (3)$$

where α is the fine-structure constant and α_i is the Dirac matrices.

The normal mass shift parameter:

$$\delta K^{\text{NMS}} = -\frac{v}{1822.888} \quad (4)$$

where 1822.888 is the ratio of atomic mass to electron mass, and v is the transition frequency. F_{ul} is related

to the total probability density of electrons:

$$F_{\text{ul}} = \frac{Z}{3\hbar} \left(\frac{e^2}{4\pi\epsilon_0} \right) \Delta |\Psi(\vec{0})|_{\text{ul}}^2 \quad (5)$$

$$\Delta |\Psi(\vec{0})|_{\text{ul}}^2 \equiv \rho_u^e(\vec{0}) - \rho_l^e(\vec{0}) \quad (6)$$

The electron density at the origin can be defined as:

$$\rho_1^e(\vec{0}) \equiv \left\langle \Psi \left| \sum_i \delta(\vec{r}_i) \right| \Psi \right\rangle \quad (7)$$

The charge distribution of the nucleus is described by a two-parameter Fermi model, and the field shift is calculated using a first-order perturbation method [24].

$$\rho(r) = \frac{\rho_0}{1 + e^{(r-c)/a}} \quad (8)$$

where ρ_0 is the normalized constant, c is the half-density radius of the nuclear charge distribution, and $a=t/(4 \ln 3)$ is related to the thickness of the nucleus.

The wavefunction, Ψ , for an atomic state in multi-configuration calculations is approximated by an atomic state function (ASF). The ASF is given as an expansion over configuration state functions.

$$\Psi(\Pi J M_J) = \sum_j c_j \Phi(\gamma_j \Pi J M_J) \quad (9)$$

where Π is the parity, J and M_J are the total angular momentum quantum number and the total magnetic quantum number, respectively. c_j is the mixing parameters and γ_j are the sets of configuration and intermediate shell-coupling quantum numbers required to unambiguously specify the configuration state functions (SCFs).

The isotope shift parameters and the electron density are calculated in a first-order perturbation approach using the multi-configuration Dirac-Hartree-Fock (MCDHF) [25–27] or relativistic configuration interaction (RCI) atomic state functions [25, 27] as the zero-order wavefunction.

For neutral atoms, the electron correlation effects play a dominate role in the discrepancies between the experimental and theoretical results. By applying restrictions on the allowed excitations, different electron correlation effects can be targeted. In this work, the electron correlation effects are evaluated by MCDHF method and Grasp2K [25] package. Nitrogen atom has four inner electrons and three valence electrons, the valance-valance correlation and inner-valance correlation are considered. The double excitations were used to carry out the calculations and the active sets are increased in a systematic way by progressively adding layers of correlation orbitals, the largest principal quantum number $n=6$ and the maximum orbital quantum number $l=g$ [28, 29].

III. RESULTS AND DISCUSSION

Grasp2K is an atomic spectroscopy calculation package based on MCDHF method. It is used to calculate Zeeman splitting, hyperfine structure, and isotope shift widely. Restricted double excitations are used in the calculation process to accelerate the convergence of the atomic wavefunction and improve the calculation efficiency and accuracy of MCDHF. In this work, all isotope shift electronic parameters of the ^{14}N and ^{15}N were calculated using the Grasp2K package interfaced with the isotope shift module Ris3 [26]. The SCF and RCI methods were used to optimize the electron wavefunction, and the Breit approximation was introduced in the RCI calculation.

The normal mass shift parameter, ΔK^{NMS} , the special mass shift parameter, ΔK^{SMS} , and F_{ul} of four multiples $3s\ 4P_{J''} \rightarrow 3p\ 4P_{J'}^{\circ}$, $3s\ 4P_{J''} \rightarrow 3p\ 4D_{J'}^{\circ}$, $3s\ 2D_{J''} \rightarrow 5p\ 2D_{J'}^{\circ}$, and $3s\ 2P_{J''} \rightarrow 3p\ 2P_{J'}^{\circ}$ are listed in Table I. The units of ΔK^{NMS} and ΔK^{SMS} are GHz·amu, that of F_{ul} is MHz/fm².

ΔK^{NMS} is calculated according to Eq.(4), and ΔK^{SMS} and F_{ul} are obtained by using the Grasp2K program. The calculated ΔK^{SMS} of two multiples, $3s\ 4P_{J''} \rightarrow 3p\ 4P_{J'}^{\circ}$ and $3s\ 4P_{J''} \rightarrow 3p\ 4D_{J'}^{\circ}$, are positive values, and those of the other two multiples, $3s\ 2D_{J''} \rightarrow 5p\ 2D_{J'}^{\circ}$ and $3s\ 2P_{J''} \rightarrow 3p\ 2P_{J'}^{\circ}$, are negative ones. All the theoretical calculated ΔK^{NMS} of those four multiples in Table I are negative values. For the multiple of $3s\ 4P_{J''} \rightarrow 3p\ 4P_{J'}^{\circ}$, the difference of ΔK^{NMS} between two transitions originated from the same lower transition level is less than 1.5 GHz·amu. However, the related difference of the ΔK^{SMS} is large and increases with the upper J values. The differences of ΔK^{SMS} and ΔK^{NMS} of the other three multiples, $3s\ 4P_{J''} \rightarrow 3p\ 4D_{J'}^{\circ}$, $3s\ 2D_{J''} \rightarrow 5p\ 2D_{J'}^{\circ}$, and $3s\ 2P_{J''} \rightarrow 3p\ 2P_{J'}^{\circ}$, are similar to that of $3s\ 4P_{J''} \rightarrow 3p\ 4P_{J'}^{\circ}$. The J value has a greater impact on ΔK^{NMS} than ΔK^{SMS} for these four multiples.

Based on ΔK^{SMS} and ΔK^{NMS} , and F_{ul} , of the N(I) atom in Table I, normal mass shifts, special mass shifts, and field shifts can be obtained. Atomic masses of ^{14}N and ^{15}N are 14.0030740074(2) and 15.000108973(12) amu [30], respectively. And the nuclear charge radii of ^{14}N and ^{15}N are 6.54285241 and 6.79175721 fm [31], respectively. The calculated SMSs, NMSs, and FSs of the $3s\ 4P_{J''} \rightarrow 3p\ 4P_{J'}^{\circ}$, $3s\ 4P_{J''} \rightarrow 3p\ 4D_{J'}^{\circ}$, $3s\ 2D_{J''} \rightarrow 5p\ 2D_{J'}^{\circ}$, and $3s\ 2P_{J''} \rightarrow 3p\ 2P_{J'}^{\circ}$ transitions are presented in Table II, and compared with experimental and theoretical values from the available literatures [16–19]. Experimental results are extracted from experimentally measured ISs. For example, the calculated SMS value of line $3s\ 4P_{1/2} \rightarrow 3p\ 4P_{3/2}^{\circ}$ is −2586.43 MHz, which is 3% smaller than the experimental one, −2505 MHz, obtained by Bai *et al.* [18], and is 5% smaller than Cangiano's result [16]. Most of our theoretical values are in agreement with Bai's recently experimental values. For the transition of $3s\ 4P_{J''} \rightarrow 3p\ 4D_{J'}^{\circ}$, our calculated SMSs are also in agree-

TABLE I Normal and specific mass shift parameters ΔK^{NMS} and ΔK^{SMS} (in GHz·amu), and field shift factor F_{ul} (in MHz/fm²) for the transitions of nitrogen.

Transitions	Transitions		ΔK^{SMS}	ΔK^{NMS}	F_{ul}
	J''	J'			
$3s\ 4P_{J''} \rightarrow 3p\ 4P_{J'}^{\circ}$	1/2	3/2	544.89	−200.80	7.04
	1/2	1/2	544.59	−200.50	6.02
	3/2	3/2	545.00	−200.24	7.04
	3/2	1/2	544.69	−199.94	6.02
	5/2	5/2	607.57	−200.11	6.33
$3s\ 4P_{J''} \rightarrow 3p\ 4D_{J'}^{\circ}$	5/2	3/2	545.16	−199.47	7.04
	1/2	1/2	515.55	−188.91	6.20
	3/2	5/2	570.91	−189.34	6.20
	3/2	1/2	515.45	−188.36	6.20
	5/2	7/2	560.93	−189.41	6.20
$3s\ 2D_{J''} \rightarrow 5p\ 2D_{J'}^{\circ}$	5/2	5/2	570.69	−188.57	6.85
	3/2	5/2	−207.80	−201.33	6.22
	3/2	3/2	−216.98	−200.46	6.21
	5/2	5/2	−207.70	−201.34	6.21
	5/2	3/2	−216.88	−200.47	6.21
$3s\ 2P_{J''} \rightarrow 3p\ 2P_{J'}^{\circ}$	1/2	1/2	−304.75	−191.31	6.26
	3/2	1/2	−304.49	−189.95	6.26

ment with the experimental values [17]. The difference between our calculation and the experiment values may be possibly due to excessive accumulation of errors during running the program. In the SCF calculation process, the average field is used to describe the interaction of particles. The average field is represented by a single-particle wavefunction. The iterative method is used to approximate the calculation to solve the nonlinear equations of the single-particle wavefunction, until the two calculation results satisfy the required precision. As a result, the total error of the results will increase in the process of iteration [25].

Based on the calculated special mass shift, normal mass shifts, and field shifts, we calculated the corresponding isotope shift of N(I), and compared them with the reported experimental results. Table III lists the theoretical calculated and experimental measured isotope shifts of $3s\ 4P_{J''} \rightarrow 3p\ 4P_{J'}^{\circ}$, $3s\ 4P_{J''} \rightarrow 3p\ 4D_{J'}^{\circ}$, $3s\ 2D_{J''} \rightarrow 5p\ 2D_{J'}^{\circ}$, and $3s\ 2P_{J''} \rightarrow 3p\ 2P_{J'}^{\circ}$ transitions. From Table III, we can see most of our calculated isotope shifts are in agreement with the reported experimental results.

For $3s\ 4P_{J''} \rightarrow 3p\ 4P_{J'}^{\circ}$ transitions, when J'' is 5/2, the maximal difference between the calculated and the experimentally measured values [16] is more than 200 MHz, and for $3s\ 4P_{J''} \rightarrow 3p\ 4D_{J'}^{\circ}$ transitions the datum of J' at 7/2 is only slightly different from the result of Holmes [15].

In our calculation, the uncertainties may come from several parts: one part is due to difference of the ab-

TABLE II Specific mass shift (SMS), normal mass shift (NMS) and field shift (FS) of N(I).

Transitions			SMS/MHz					NMS/MHz	FS/MHz
	J''	J'	This work	Expt. [18]	Calc. [19]	Calc. [17]	Expt. [14, 16]	This work	This work
3s $^4P_{J''} \rightarrow 3p \ ^4P_{J'}$	1/2	3/2	-2586.43	-2505(27)			-2457(150) [16]	953.14	1.75
	1/2	1/2	-2584.99	-2479(14)				951.70	1.50
	3/2	3/2	-2586.94	-2609(3)			-2503(150) [16]	950.50	1.75
	3/2	1/2	-2585.50	-2561(14)	-2579.4(68)	-2558.3(22)	-2555(150) [16]	949.07	1.50
	5/2	5/2	-2883.95	-2714(10)	-2745.4(18)	-2745.4(18)	-2733(150) [16]	949.85	1.58
	5/2	3/2	-2587.69	-2755(10)	-2746.4(17)	-2713.4(14)	-2843(150) [16]	946.85	1.75
	3/2	1/2	-2447.17	-2465(6)	-2488.1(15)	-2488.1(15)		896.71	1.54
3s $^4P_{J''} \rightarrow 3p \ ^4D_{J'}$	3/2	5/2	-2709.93	-2562(10)				898.76	1.54
	3/2	1/2	-2446.71	-2566(27)				894.08	1.54
	5/2	7/2	-2662.57	-2749(10)	-2746.4(18)	-2762.9(16)		899.08	1.54
	5/2	5/2	-2708.89	-2736(10)	-2748.17(84)	-2748.17(84)		895.11	1.71
	5/2	3/2	1029.46					951.58	1.54
3s $^2D_{J''} \rightarrow 5p \ ^2D_{J'}$	3/2	5/2	986.38	917(21)				955.64	1.55
	3/2	3/2	1029.96	1146(45)				951.54	1.55
	5/2	5/2	985.88	1016(18)				955.68	1.54
	5/2	3/2	1029.46					951.58	1.54
3s $^2P_{J''} \rightarrow 3p \ ^2P_{J'}$	1/2	1/2	1446.58				1341(18) [14]	908.11	1.56
	3/2	1/2	1445.33				1449(42) [14]	901.62	1.56

TABLE III Summary of the isotope shifts of ^{14}N and ^{15}N . The reference isotope is ^{14}N .

Transitions			SMS/MHz				
	J''	J'	This work	Expt. [18]	Calc. [17]	Calc. [16]	Calc. [14, 15]
3s $^4P_{J''} \rightarrow 3p \ ^4P_{J'}$	1/2	3/2	-1631.54	-1549(27)		-1518(150)	-1500(300)
	1/2	1/2	-1631.79	-1524(14)			-1500(300)
	3/2	3/2	-1634.68	-1655(3)	-1557(150)	-1500(300)	
	3/2	1/2	-1634.93	-1609(14)	-1609.3(22)	-1610(150)	-1800(180)
	5/2	5/2	-1932.52	-1761(10)	-1795.6(18)	-1788(150)	-1732(15)
	5/2	3/2	-1639.09	-1805(10)	-1766.6(14)	-1901(150)	-1788(18)
3s $^4P_{J''} \rightarrow 3p \ ^4D_{J'}$	1/2	1/2	-1548.92	-1565(6)	-1591.4(15)		-1800(300)
	3/2	5/2	-1809.63	-1660(10)			
	3/2	1/2	-1551.09	-1669(27)			
	5/2	7/2	-1761.94	-1847(10)	-1863.8(16)		
	5/2	5/2	-1812.08	-1838(10)	-1853.0(84)		-1800(300)
3s $^2D_{J''} \rightarrow 5p \ ^2D_{J'}$	3/2	5/2	1943.57	1876(21)			
	3/2	3/2	1983.04	2101(45)			
	5/2	5/2	1943.10	1975(18)			
	5/2	3/2	1982.58				
3s $^2P_{J''} \rightarrow 3p \ ^2P_{J'}$	1/2	1/2	2356.25				2253(18)
	3/2	1/2	2348.51				2355(42)

solute transition frequency that is used in the Eq.(4) to calculate the normal mass shift parameter. Absolute uncertainties in our work are about 2.8 MHz, and the effect on IS is around 0.1%. In our calculation, the largest principal quantum number was set to $n=6$, the uncertainty due to the atomic orbitals could not be included entirely, and the contribution from this part is

$\sim 0.1\%$ [28]. In the calculation, the atomic weight is used to replace the nuclear mass, which introduces new errors. The weights of the nucleus can be corrected by the following expression [32]:

$$M_{\text{nuclear}} = M_{\text{atom}} - Z_{m_e} + B_{\text{el}} \quad (10)$$

where, M_{nuclear} is the nucleus mass, M_{atom} is the atomic

weight, m_e is the electron weights, and B_{el} is the binding energy. The calculation error caused by the MCDHF method in the calculation can introduce quantum electrodynamics (QED) correction to improve the accuracy [33].

IV. CONCLUSION

We theoretically calculated the isotope shift parameters, ΔK^{SMS} and ΔK^{NMS} , of four multiples ($3s\ 4P \rightarrow 3p\ 4P^\circ$, $3s\ 4P \rightarrow 3p\ 4D^\circ$, $3s\ 2D \rightarrow 5p\ 2D^\circ$, and $3s\ 2P \rightarrow 3p\ 2P^\circ$) of ^{14}N and ^{15}N using the Grasp2K program and the Ris3 package, and obtained the SMS, NMS, FS, and IS values of these transitions. And compared with the reported experimental ones, most of our calculated results are in agreement with the experimental values. However, the difference for some transitions is large, around 7%. We also discussed the possible reasons which led to these large difference. The theoretical calculation method need to be developed for more accurate results to help scientists to do experiment investigation.

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