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Reanalysis of the even configurations system of atomic niobium

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ABSTRACT

In this work a reanalysis of the even configurations system of atomic niobium (Nb I) is presented.

A multiconfiguration parametric calculation on the basis of 14 even configurations have been performed by taking into account the second-order of the perturbation theory. Satisfactory consistency of the values of experimental and calculated energy levels, Landé g_J factors and hyperfine structure constants was found in most cases. New experimental data, recently published, allowed to obtain more reliable wavefunctions and to predict the energy levels values and the hyperfine structure constants, if no experimental values are available.

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1. Introduction

Niobium, formerly known as Columbium, is a representative of the 4d shell transition group elements. The only stable ^{93}Nb isotope, due to the large nuclear magnetic dipole moment, shows a broad hyperfine structure (hfs). As a neutron-capture element, niobium plays an important role in the investigations of the nucleosynthesis of heavy elements. The broad hyperfine structure pattern can affect the abundances values deduced from the equivalent widths of stellar lines [1]. Therefore, the knowledge of hyperfine splitting of the spectral lines, also those predicted, is particularly important.

The early observations of Nb I spectra took place in the 20s and 30s of the previous century [2–4]. During this period, the first observations of the hyperfine structure and nuclear moments estimation were also presented [5]. Research in this area was continued in the following years [6–8].

The development of precise spectroscopic methods, such as atomic-beam magnetic-resonance, laser and radio-frequency spectroscopic methods, Doppler-limited optogalvanic spectroscopy and Doppler-reduced saturation spectroscopy, allowed for extensive experimental investigation of the Nb I hyperfine structure [9–17]. In recent years, high-resolution Fourier transform spectroscopy measurements of Nb I were presented [18–21].

Theoretical studies of the fine and hyperfine structures were published by Büttgenbach and Dicke in 1975 [22], Büttgenbach in 1982 [23], Kröger and Bouzed in 2003 [24] and by Kröger et al. in 2007 [25].

In 2015 we presented a parametric study of the fine and hyperfine structure for the even parity configurations of atomic niobium [26], as a result of a large amount of new experimental data. A multiconfiguration fit of 14 configurations was performed, taking into account the second-order of the perturbation theory including the effects of closed-open shell excitations. The experimental data available at that time have been enriched by predicted values of energies, Landé g_J-factors and hfs A and B constants, obtained by means of the applied semi-empirical procedure. As we mentioned in the conclusions, the accuracy of predictions would increase if more experimental data become available. Therefore, new experimental results reported by Kröger et al. [27] and by Windholz and Kröger [28] motivated us to reanalyze the fine and hyperfine structure of atomic niobium, presented in the current paper.

Already the preliminary analysis of the predicted energy levels and hyperfine structure constants published in our previous paper [26], indicates that new levels [27] in the energy range around 40,000–41,000 cm^{-1} can be assigned to ^{4}F states of 4d^{3}5s6s configuration, whereas the levels of about 43,000 cm^{-1} with small negative or positive magnetic dipole constants to states of 4d^{4}5d and 4d^{3}5s5d configurations, respectively. Therefore, the reanalysis will allow us to more reliable determination of the center of gravity above mentioned configurations. Additionally, the corrected value of hfs A constant for the level 23,010.58 cm^{-1}, $J = 9/2$ [28] is in better compliance with our prediction.

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Table 1
Values of the fine structure radial parameters [cm^{-1}]. (*) denotes **a** fixed parameter, [a] denotes arbitrarily assumed value of the center of gravity of the configuration, (**) denotes the parameters common for all configurations. The values of ab-initio radial parameters were given also for comparison.

Parameter	Value		HFR [40]
$E_{AV}(4d^5)$	30,796	(52)	36,761
$F^2(4d,4d)$	53,550	(280)	(**)
$F^4(4d,4d)$	33,377	(180)	(**)
$\zeta(4d)$	759	(38)	(**)
$D^0(3d4d,4d4d)$ $\zeta_{3d,\,4d}$	−42.2	(5.2)	
$D^2(3d4d,4d4d)$ $\zeta_{3d,\,4d}$	−34	(17)	
$D^0(3d4d,4d4d)$ $D^2(3d4d,4d4d)$	−1292	(17)	
$D^0(3d4d,4d4d)$ $D^4(3d4d,4d4d)$	−718	(*)	
$D^2(3d4d,4d4d)$ $D^2(3d4d,4d4d)$	−550	(210)	
$D^2(4d4d,5d5d)$ $D^2(4d4d,5d5d)$	2520	(230)	
$D^2(n_0s4d,4d4d)$ $D^2(n_0s4d,4d4d)$	−550	(210)	
$D^1(n_0pn_0p,4d4d)$ $D^1(n_0pn_0p,4d4d)$	2460	(130)	
$E_{AV}(4d^45s)$	18,727	(28)	21,202
$G^2(4d,5s)$	11,989	(77)	10,819
$E^2(3d5s,5s4d)$ $\zeta_{3d,\,4d}$	44	(22)	
$E^2(3d5s,5s4d)$ $E^2(3d5s,5s4d)$	3240	(180)	
$E_{AV}(4d^46s)$	52,395	(31)	53,580
$G^2(4d,6s)$	2071	(46)	1208
$E_{AV}(4d^45d)$	56,096	(*)	58,067
$F^2(4d,5d)$	2360	(*)	1656
$\zeta(5d)$	55	(*)	25
$E_{AV}(4d^35s^2)$	17,770	(52)	17,770[a]
$E_{AV}(4d^35s6s)$	53,805	(38)	52,638
$G^0(5s,6s)$	721	(36)	1000
$E_{AV}(4d^35s5d)$	58,285	(*)	58,185
$4d^5 \leftrightarrow 4d^45s$			
$R^2(4d4d,4d5s)$	−13,920	(140)	−13,742
$D^1(n_0pn_0p,4d5s)D^1(n_0pn_0p,4d4d)$	−1740	(470)	

2. Semi-empirical analysis of experimental data

In the current work we investigated the atomic structure of the even-parity configurations system of niobium using a semi-empirical parametrization method, which allows the analysis of a complex electronic system, taking into account all electromagnetic interactions in an atom up to the second-order perturbation theory [29–38]. Our computer procedures lead to determination of precise wave functions for each electronic state. The wave functions can be used to predict the values of energy levels, g_j-Landé factors and hyperfine structure constants, if sufficient experimental data are available. The agreement between the expected and experimentally determined values is the test of correctness of the eigenvectors amplitudes.

As in the previous work [26], we considered a system of 14 configurations: $4d^5$, $4d^4n's$ (n′=5,6), $4d^45d$, $4d^45g$, $4d^35s^2$, $4d^35s6s$, $4d^35s5d$, $4d^35s5g$, $4d^35p^2$, $4d^25s5p^2$, $4d^25s^26s$, $4d^25s^25d$ and $4d^25s^25g$. The considered system is described by means of 1927 fine structure radial parameters, reduced by applying the relations based on the effective quantum numbers to 746 parameters. Additionally, the radial parameters of the same type, involving the same electrons are assumed to be the same for all considered configurations. Finally, only 23 parameters were fitted as free parameters.

The values of the fine structure radial parameters, together with their statistical errors, are presented in Table 1, resulting from a fit of the 84 experimentally known energy levels with mean deviation of 29 cm^{-1}. Most of the parameters were not fitted but fixed on theoretical Hartree–Fock values [39,40], and remained unchanged compared to the previous work [26]. Thus Table 1 gives only parameters changed in relation to those in the Tables 3 and 4 at that work.

The hyperfine structure parametrization was conducted with the use of 757 and 385 radial parameters for the magnetic dipole and the electric quadrupole hfs interactions, respectively. The number of fitted parameters was reduced to 15 for the A constants and 9 for the B constants. In our analysis we considered 84 A constants and 34 B constants, respectively. The values obtained by means of atomic-beam magnetic-resonance [9] or laser and radio-frequency spectroscopic methods [10] were taking to calculations with three times higher statistical weight. In the case of electric quadrupole constants, 11 from the total number of 44, with a large relative experimental uncertainty, were not included. Mean deviations of 19 and 10 MHz for A and B constants, respectively, were achieved. The hyperfine structure radial parameters, together with their root mean square errors, are given in Table 2.

Table 2
One- and two-body hyperfine structure radial parameters [MHz] for the even parity configurations of Nb I.

Parameter	Value		Comments
Magnetic-dipole hfs interactions			
$a^{01}_{4d} = a^{12}_{4d}$	446.4	(9.3)	Fitted
a^{10}_{5s}	5750	(390)	Fitted
a^{10}_{6s}	1243	(85)	$a^{10}_{6s} = 0.216a^{10}_{5s}$
$a^{01}_{5d} = a^{12}_{5d}$	81	(54)	Fitted
$D^0(3d\ 4d,\ 4d\ 4d)\ P^{01}(3d,4d) =$	−13.6	(1.3)	Fitted
$D^0(3d\ 4d,\ 4d\ 4d)\ P^{12}(3d,4d)$	−18.6	(2.1)	Fitted
$D^2(3d\ 4d,\ 4d\ 4d)\ P^{01}(3d,4d) =$			
$D^2(3d\ 4d,\ 4d\ 4d)\ P^{12}(3d,4d)$	−51.2	(8.0)	Fitted
$D^4(3d\ 4d,\ 4d\ 4d)\ P^{01}(3d,4d) =$			
$D^4(3d\ 4d,\ 4d\ 4d)\ P^{12}(3d,4d)$	−28.4	(4.4)	$D^4/D^2 = 0.55556$
$E^2(n_0s4d,\ 4d\ 5s)\ P^{10}(n_0s,5s)$	−1284	(10)	Fitted, $n_0 = 1,\ldots,4$
$E^2(n_0s4d,\ 4d\ 6s)\ P^{10}(n_0s,6s)$	−277	(2)	$P^{10}(6s)/P^{10}(5s) = 0.216$
$E^2(n_0s4d,\ 4d\ 7s)\ P^{10}(n_0s,7s)$	−101	(1)	$P^{10}(7s)/P^{10}(5s) = 0.0787$
			$n_0 = 1,\ldots,5$
$E^2(3d\ 5s,\ 5s\ 4d)\ P^{01}(3d,4d) =$			
$E^2(3d\ 5s,\ 5s\ 4d)\ P^{12}(3d,4d)$	16	(9)	Fitted
$D^0(n_0s4d,\ 5s\ 4d)\ P^{10}(n_0s,5s)$	−473	(31)	Fitted, n_0=1,...,4
$D^0(n_0s5s,\ 5s\ 5s)\ P^{10}(n_0s,5s)$	1667	(91)	Fitted, n_0=1,...,4
$E^2(n_0s4d,\ 4d\ 6s)\ P^{10}(n_0s,6s)$	189	(18)	Fitted, n_0=1,...,5
$a^{12}_{4d.5s}$	169	(18)	Fitted
$D^2(3d\ 4d,\ 4d\ 5s)\ P^{01}(3d,4d) =$			
$D^2(3d\ 4d,\ 4d\ 5s)\ P^{12}(3d,4d)$	35	(24)	Fitted
$E^2(3d\ 4d,\ 5s\ 4d)\ P^{01}(3d,4d) =$			
$E^2(3d\ 4d,\ 5s\ 4d)\ P^{12}(3d,4d)$	−21	(27)	Fitted
$D^2(n_0s4d,\ 4d\ 4d)\ P^{10}(n_0s,5s)$	3564	(49)	Fitted, n_0=1,...,4
Electric-quadrupole hfs interactions			
b^{02}_{4d}	−365	(31)	Fitted
b^{13}_{4d}	−102	(19)	Fitted
b^{11}_{4d}	19	(10)	Fitted
$D^0(3d\ 4d,\ 4d\ 4d)\ P^{02}(3d,4d)$	23	(5)	Fitted
$D^2(3d\ 4d,\ 4d\ 4d)\ P^{02}(3d,4d)$	31	(14)	Fitted
$D^4(3d\ 4d,\ 4d\ 4d)\ P^{02}(3d,4d)$	17	(8)	$D^4/D^2 = 0.55556$
$b^{02}_{4d.5s}$	83	(20)	Fitted
$D^2(3d\ 4d,\ 4d\ 5s)\ P^{02}(3d,4d)$	287	(54)	Fitted
$E^2(3d\ 4d,\ 5s\ 4d)\ P^{02}(3d,4d)$	283	(61)	Fitted
$D^2(3d\ 5s,\ 4d\ 4d)\ P^{02}(3d,4d)$	77	(39)	Fitted

The combined result of the fine- and hyperfine structure calculations is presented in Table 3. The first three columns present the values of experimantal and calculated energy values of electronic levels and the difference between them in cm^{-1}. The two main fine structure components with their percentages, are given in columns 4–7. In next columns (8 and 9), the calculated g_J values are compared with the experimental ones. In columns 10 and 12 the experimental hyperfine constants A and B are listed together with their experimental uncertainties. The calculated A and B constants for all energy levels are listed in columns 11 and 13. In the last column (14), the references to experimental hfs constants are given. The energy and g_J values were taken from the NIST Atomic Spectra Database [41], except those with the reference [20], [27] or [42] in the last column.

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