

Comparative Studies on Russell-Saunders Atomic Term Symbols (Terms) for Equivalent Electrons of nf^4 and nf^{10} Configurations

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There are two coupling schemes for obtaining Russell Saunders atomic term symbols (terms) for the equivalent electrons, one is Russell-Saunders (L-S) coupling scheme and another is spin-orbit (j-j) coupling scheme. The Russell Saunders atomic term symbol provide the information about spectral and magnetic properties of an atom. For this work computation is done to calculate all the possible microstates and atomic terms for equivalent electrons of nf^4 and nf^{10} configurations and a comparative study is carried out between the Russell Saunders atomic terms of nf^4 and nf^{10} configurations. The possible microstates counted for these configurations are 1001 and the terms obtained from these states are 47, these terms are quintets (5), triplets (22) and singlet's (20) and the predicted ground state term for both the configurations is quintet I (⁵I). The ground states for nf^4 and nf^{10} configuration are ⁵I₄ and ⁵I₈ respectively.

Key-words: Term symbol, Russell-Saunders term, Microstate, Singlet, Triplet and Quintet.

INTRODUCTION

The Russell –Saunders (L-S) coupling scheme first proposed by Henry Russell and Frederick Saunders in 1923 [1] and originally used for electrons in partially filled shells of elements with lower atomic number but for the elements with greater atomic number spin-orbit coupling becomes more significant because higher nuclear charge [2-4]. However, for heavier transition elements and rare earth elements it is still convenient to use Russell-Saunders scheme [5]. The vector model for terms which was developed before the quantum mechanical treatment was successfully used to interpret the complex spectra of systems with valence electrons in different sub shells [6]. The current nomenclature for the various energy levels (^{2S+1}L) is based on the Russell–Saunders coupling which leads to the three vectors \vec{S} , \vec{L} and \vec{J} . \vec{L} is the vectorial sum of the orbital angular momentum vectors of the valence electrons, \vec{S} is the vectorial sum of the spin angular momentum vectors of the valence electrons and \vec{J} is the vectorial sum of \vec{L} and \vec{S} . L and S coupled together to give a state of definite J [7] and the allowed values of J range from L+ S to |L-S|. The each term split into (2J+1) terms differing in energy by an amount proportional

to the applied field strength (Zeeman effect) and states are characterized by a quantum number M_J which have allowed values of J, J-1..., -J+1, -J [8]. It follows that if $L \geq S$ the J can take 2S+1 values, but if $L < S$ it can take 2L+1 values, when $L=0$ J can take only one value. The values of J may be either 1+1/2 or 1-1/2 but 1-1/2 is of lower energy state since in 1-1/2 state the orbital and spin are opposed [9, 10] By knowing the allowed values of L, S and J one can define the energy levels for the valence electrons [11].

A Russell-Saunders atomic term is applied for energy associated with the state of an atom involved in a transition and term symbols are abbreviated description of the energy levels in a multi electron atom. The degenerated state is broken up into two or more states due to electronic repulsion when the ion or atom is introduced into a lattice [12]. The equivalent electrons are those which have same values of l such as np^2 , nd^4 , nf^2 or nf^5 configuration. The formulation of hole can be used for the sub shell that is more than half full and the equivalent electrons for a pair of atoms with n^m and n^{x-n} ($x=6, 10$ or 14) configurations give rise identical Russell Saunders atomic term symbols [13]. Therefore, the equivalent electrons of nf^4 and nf^{10} configurations give identical terms. The numbers of microstates for the incomplete sub shell increase with increase in the number of electrons in orbital of the sub shell but in the nonequivalent electronic system the number of microstates are

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much greater than the similar equivalent electronic system [14]. In the Russell Saunders coupling a term is specified by $(2S+1)L_J$ [2, 3, 7, 10] where $2S+1$ the multiplicity or spin multiplicity of a term. The number of states deriving from a given term is simply $(2S+1) \times (2L+1)$ and the stability order and ground state term can be predicted by applying Hund's rule [5, 10-15].

The problem with equivalent d or f electrons or nonequivalent electrons is finding the microstates, which are 252 for nd^5 , 364 for nf^3 , 1001 for nf^4 , 2002 for nf^5 , 3003 for nf^6 and 3442 for nf^7 for equivalent electrons and for nonequivalent electrons 910 for $f^2 d^1$, 3640 for $f^3 d^1$ and 10010 for $f^4 d^1$. Methods have been introduced to help generate the states [16, 17] and used for cases up to nd^5 for equivalent electrons. The Russell Saunders terms have been determined for equivalent electrons of nf^3 and nf^{11} configuration [18, 19] and for nonequivalent electrons of $f^2 d^1$ configuration using R-S coupling scheme [20].

METHODOLOGY

Counting Total number of Microstates for nf^4 and nf^{10} configurations

The total number of microstates for any configuration can be counted using by following expression [21].

Number of ways of filling electrons $N = \frac{2(2l+1)!}{x!(2(2l+1)-x)!}$ or $\frac{n!}{x!(n!-x)!}$ (1)

$n = 2(2l+1)$ or double of the total number of orbital's, $x =$ Total number of electrons in sub shell. So, for nf^4 configuration $n = 2(2l+1) = 14$ and $x = 4$ and for nf^{10} configuration $n = 2(2l+1) = 14$ and $x = 10$.

For nf^4 configuration $N = \frac{14!}{4!(14!-4!)}$ and for

nf^{10} configuration $N = \frac{14!}{10!(14!-4!)}$

$N = \frac{14 \times 13 \times 12 \times 11 \times 10 \times 9 \times 8 \times 7 \times 6 \times 5 \times 4 \times 3 \times 2 \times 1}{4 \times 3 \times 2 \times 1 \times 10 \times 9 \times 8 \times 7 \times 6 \times 5 \times 4 \times 3 \times 2 \times 1}$

Therefore, $N = 1001$ Microstates for nf^4

$N = \frac{14 \times 13 \times 12 \times 11 \times 10 \times 9 \times 8 \times 7 \times 6 \times 5 \times 4 \times 3 \times 2 \times 1}{4 \times 3 \times 2 \times 1 \times 10 \times 9 \times 8 \times 7 \times 6 \times 5 \times 4 \times 3 \times 2 \times 1}$

Therefore, $N = 1001$ Microstates for nf^{10}

Counting the values for Total Orbital Angular Momentum Quantum Number (L), Total Spin Angular Momentum Quantum Number (S), M_L , M_S and J

Therefore, L values for nf^4 and nf^{10} configurations are 0,1,2,3,4,5,6,7,8,9 and 10 and the

atomic terms codes for these L values are S, P, D, F, G, H, I, K, L, M and N.

The length of total orbital angular momentum vector \vec{L} is $|\vec{L}| = \sqrt{L(L+1)} \hbar$. (3)

Therefore, $|\vec{L}|$ are $\sqrt{110} \hbar, \sqrt{90} \hbar, \sqrt{72} \hbar, \sqrt{56} \hbar, \sqrt{42} \hbar, \sqrt{30} \hbar, \sqrt{20} \hbar, \sqrt{12} \hbar, \sqrt{6} \hbar, \sqrt{2} \hbar$ and 0.

$\vec{S} = (s_1+s_2), (s_1+s_2-1) \dots, (s_1-s_2) |$. (4)

Therefore, \vec{S} vectors are for nf^4 and nf^{10} configurations are 2, 1 or 0.

Therefore, \vec{S} vector length is $|\vec{S}| = \sqrt{S(S+1)} \hbar$. (5)

Therefore, for nf^4 and nf^{10} configurations of \vec{S} vectors are $\sqrt{6} \hbar, \sqrt{2} \hbar$ and zero.

The component of the total angular momentum along a given axis is $M_L = 2L + 1$ (6)

Here $L = 10$ (maximum value of L for nf^4 and nf^{10} configurations), Therefore, $M_L = 2 \times 10 + 1 = 21$ values that ranging from +10 to -10.

The spin state for a given S value is

$M_S = (2S + 1)$ (7)

Here $S = 2$ (maximum value of S for nf^4 and nf^{10} configurations), Therefore, $M_S = 2 \times 2 + 1 = 5$ values that ranging from +2 to -2.

Therefore, J values for 3M term are 10, 9 and 8 and other terms illustrated in table 5 Magnitude of vector sum of L and S or magnitude of J is $\sqrt{J(J+1)} \hbar$ (8)

The vectorial sums for L and S for some terms are illustrated in figure 1.

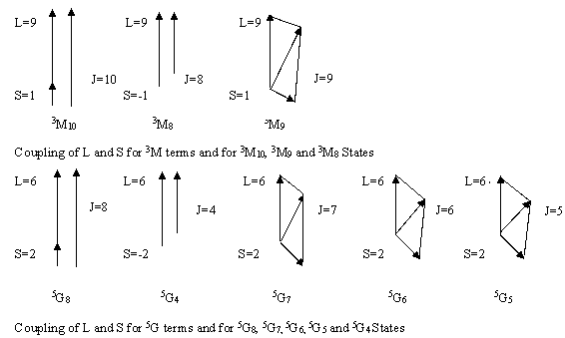


Figure 1: L-S coupling for J values for different terms and states

The Fundamental Tables for Russell Saunders Coupling Scheme

The fundamental table for equivalent electrons for nf^4 configuration (table 1) and for nf^{10} (table 2) configuration for Russell Saunders coupling scheme representing possible spin states that allowed by the Pauli Principle with the microstates. These tables include total number of microstates with spin states. The fundamental table 3

Table 1: The fundamental table for equivalent electrons of nf^4 configuration used in Russell Saunders coupling scheme representing possible spin states that allowed by the Pauli Principle with microstates.

S.N.	Possible spin states for nf^4 electrons				Total spin	Total microstates
1	↑	↑	↑	↑	+2	35
2	↑	↑	↑	↓	+1	140
3	↑	↑	↓	↓	0	210
4	↑	↓	↓	↓	-1	140
5	↓	↓	↓	↓	-2	35
6	↑↓	↑	↑		+1	105
7	↑↓	↑	↓		0	210
8	↑↓	↓	↓		-1	105
9	↑↓	↑↓			0	21

Total number of microstates for nf^4 configuration -1001

Table 2: The fundamental table for equivalent electrons of nf^{10} configuration used in Russell Saunders coupling scheme representing possible spin states that allowed by the Pauli Principle with microstates.

S.N.	Possible spin states for nf^{10} electrons						Total spin	Total microstates
1	↑↓	↑↓	↑↓	↑	↑	↑	+2	35
2	↑↓	↑↓	↑↓	↑	↑	↓	+1	140
3	↑↓	↑↓	↑↓	↑	↑	↓	0	210
4	↑↓	↑↓	↑↓	↑	↓	↓	-1	140
5	↑↓	↑↓	↑↓	↓	↓	↓	-2	35
6	↑↓	↑↓	↑↓	↑	↑		+1	105
7	↑↓	↑↓	↑↓	↑	↓		0	210
8	↑↓	↑↓	↑↓	↓	↓		-1	105
9	↑↓	↑↓	↑↓	↑↓			0	21

Total number of microstates for nf^{10} configuration - 1001

Table 3: The fundamental table representing total microstate numbers according to M_L and M_S valufor equivalent electrons of nf^4 and nf^{10} configurations.

$M_S \rightarrow$	+2	+1	0	-1	-2	Total
10			1			1
9		1	2	1		4
8		2	5	2		9
7		4	8	4		16
6	1	7	14	7	1	30
5	1	11	20	11	1	44
4	2	15	28	15	2	62
3	3	20	34	20	3	80
2	4	23	41	23	4	95
1	4	26	44	26	4	104
↑ M_L	5	27	47	27	5	111
-1	4	26	44	26	4	104
-2	4	23	41	23	4	95
-3	3	20	34	20	3	80
-4	2	15	28	15	2	62
-5	1	11	20	11	1	44
-6	1	7	14	7	1	30
-7		4	8	4		16
-8		2	5	2		9
-9		1	2	1		4
-10			1			1
Total	35	245	441	245	35	1001

representing microstate numbers according to M_L and M_S values for equivalent electrons for nf^4 and nf^{10} configurations and table 4 representing microstate array M_L versus $2S+1$ in a statistical way for both the configurations

Resolving the Microstate Chart into Appropriate Atomic States and Drawing Sub Tables for Each Terms

An atomic state forms an array of microstate consisting $2S+1$ columns and $2L+1$ rows. Thus, for a 3N state requires two columns or (21×3) array, 3M state requires (19×3) array and 5L state requires (15×5) array¹⁰. By removing each state from the microstate table a microstate sub table for each Russell Saunders term can be drawn. This treatment on microstates for both nf^4 and nf^{10} configurations give 5I , 5G , 5F , 5D , 5S , 3M , 3L , $^3K(2)$, $^3I(2)$, $^3H(4)$, $^3G(3)$, $^3F(4)$, $^3D(2)$, $^3P(3)$, 1N , $^1L(2)$, 1K , $^1I(3)$, $^1H(2)$, $^1G(4)$, 1F , $^1D(4)$ and $^1S(2)$ atomic terms. The microstates of electrons remain conserved in atomic terms, therefore, it is verified by obtaining the microstates from the atomic terms and it is given in table 5.

Stability and splitting pattern of Russell- Saunders Atomic Terms

The splitting pattern and stability order of Russell- Saunders atomic terms for equivalent or non-equivalent electrons for a particular configuration can be predicted by applying Hund's rule. For the nf^4 and nf^{10} configuration it is illustrated in (figure1) and this splitting pattern give different ground states for nf^4 and nf^{10} configurations, since one (nf^4) has less than half fill orbital configuration and another (nf^{10}) has more than half fill orbital configuration.

RESULT AND DISCUSSION

There are the three types of Russell Saunders atomic terms obtained from the microstates for equivalent electrons of nf^4 and nf^{10} configurations that are quintets (5), triplets (22) and singlet's (20). These terms are 5I , 5G , 5F , 5D , 5S , 3M , 3L , $^3K(2$ -Terms), $^3I(2$ -Terms), $^3H(4$ -Terms), $^3G(3$ -Terms), $^3F(4$ -Terms), $^3D(2$ -Terms), $^3P(3$ -Terms), 1N , $^1L(2$ -Terms), 1K , $^1I(3$ -Terms), $^1H(2$ -Terms), $^1G(4$ -Terms), 1F , $^1D(4$ -Terms) and $^1S(2$ -Terms). The ground state term for both the configurations obtained is Quintet I (5I).

CONCLUSION

It is concluded that the equivalent electrons of nf^4 and nf^{10} configurations can be arranged in 1001

$M_S \rightarrow$	+2	+1	0	-1	-2	Total
10						1
9						4
8						9
7						16
6						30
5						44
4						62
3						80
2						95
1						104
$\uparrow M_L 0$						111
-1						104
-2						95
-3						80
-4						62
-5						44
-6						30
-7						16
-8						9
-9						4
-10						1
Total	35	245	441	245	35	1001

Table 4: The fundamental table representing microstate array M_L v/s $2S+1$ in a statistical way for equivalent electrons of nf^4 and nf^{l0} configurations.

S.N.	Term symbol	Total values of J	Several Possible Terms	Array	Micro States
1	1N	J=1	$^1N_{10}$	21x1	21
2	3M	J=3	$^3M_{10}, ^3M_9, ^3M_8$	19x3	57
	3L	J=3	$^3L_9, ^3L_8, ^3L_7$	17x3	51
3	$^1L(2)$	J=1	1L_8	(17x1)2	34
4	$^3K(2)$	J=3	$^3K_8, ^3K_7, ^3K_6$	(15x3)2	90
	1K	J=1	1K_7	15x1	15
	5I	J=5	$^5I_8, ^5I_7, ^5I_6, ^5I_5, ^5I_4$	13x5	65
5	$^3I(2)$	J=3	$^3I_7, ^3I_6, ^3I_5$	(13x3)2	78
	$^1I(3)$	J=1	1I_6	(13x1)	39
6	$^3H(4)$	J=3	$^3H_6, ^3H_5, ^3H_4$	(11x3)4	132
	$^1H(2)$	J=1	1H_5	(11x1)2	22
	5G	J=5	$^5G_6, ^5G_5, ^5G_4, ^5G_3, ^5G_2$	9x5	45
7	$^3G(3)$	J=3	$^3G_5, ^3G_4, ^3G_3$	(9x3)3	81
	$^1G(4)$	J=1	1G_4	(9x1)4	36
	5F	J=5	$^5F_5, ^5F_4, ^5F_3, ^5F_2, ^5F_1$	7x5	35
8	$^3F(4)$	J=3	$^3F_4, ^3F_3, ^3F_2$	(7x3)4	84
	1F	J=1	1F_3	7x1	7
	5D	J=5	$^5D_4, ^5D_3, ^5D_2, ^5D_1, ^5D_0$	5x5	25
9	$^3D(2)$	J=3	$^3D_3, ^3D_2, ^3D_1$	(5x3)2	30
	$^1D(4)$	J=1	1D_2	(5x1)4	20
10	$^3P(3)$	J=3	$^3P_2, ^3P_1, ^3P_0$	(3x3)3	27
	5S	J=1	5S_2	1x5	5
11	$^1S(2)$	J=1	1S_0	(1x1)2	2
Total number of microstates for nf^4 and nf^{l0} configuration-1001					

Table 5: Conservation of state or levels a cross verification of terms and microstates for equivalent the electrons of nf^4 and nf^{l0} configurations.

energy states or levels that have different values of s (spin quantum numbers) and l (angular quantum numbers) and 47 Russell-Saunders atomic spectroscopic terms symbols (terms) obtained from

these states by R-S coupling treatment. Theoretical stability order of these Russell-Saunders atomic terms according to Hund's rule is

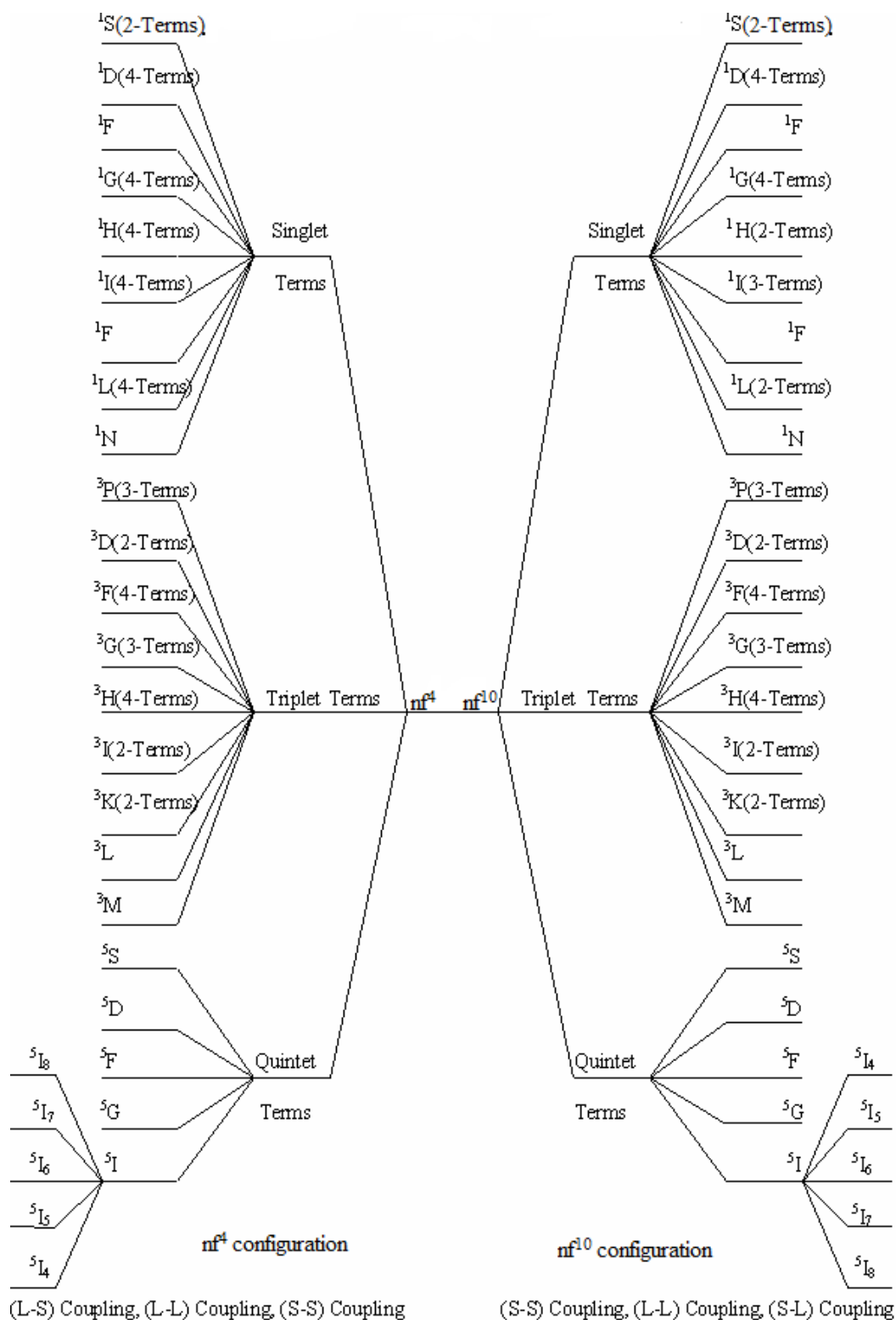


Fig. 2: The stability order and splitting pattern of Russell-Saunders atomic terms for equivalent the electrons for nf^4 and nf^{10} configurations.

$^5I > ^5G > ^5F > ^5D > ^5S > ^3M > ^3L > ^3K(2) > ^3I(2) > ^3H(4) > ^3G(3) > ^3F(4) > ^3D(2) > ^3P(3) > ^1N > ^1L(2) > ^1K > ^1I(3) > ^1H(2) > ^1G(4) > ^1F > ^1D(4) > ^1S(2)$ and the stability order of ground state terms for nf^4 configuration is $^5I_8 < ^5I_7 < ^5I_6 < ^5I_5 < ^5I_4$ and for nf^{10} is $^5I_8 > ^5I_7 > ^5I_6 > ^5I_5 > ^5I_4$. This study illustrates that equivalent electrons for nf^4 and

nf^{10} configurations give same type of atomic terms and same number microstates but the ground states for both configurations are different, since nf^4 configuration has less than half fill orbital configuration while nf^{10} configuration has more than half fill orbital configuration. Therefore, the

ground state for nf^4 configuration is quintet I four (5I_4) and for nf^{10} configuration is quintet I eight (5I_8).

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Supplementary Data

The fundamental sub tables for each Russell Saunders atomic terms for equivalent electrons of nf^4 and nf^{10} configurations.

M_s	0
10	
9	
8	
7	
6	
5	
4	
3	
2	
1	
M_L0	
-1	
-2	
-3	
-4	
-5	
-6	
-7	
-8	
-9	
-10	
21	

$L=10, S=0, 2S+1=1, \text{Microstates}=21, \text{Term}={}^1N$

M_s	+1	0	-1
9			
8			
7			
6			
5			
4			
3			
2			
1			
M_L0			
-1			
-2			
-3			
-4			
-5			
-6			
-7			
-8			
-9			
	19	19	19

$L=9, S=1, 2S+1=3, \text{Microstates}=57, \text{Term}={}^3M$

M_S	+1	0	-1
8			
7			
6			
5			
4			
3			
2			
1			
$M_L 0$			
-1			
-2			
-3			
-4			
-5			
-6			
-7			
-8			
	17	17	17

L=8, S=1, 2S+1=3, Microstates=51, Term= 3L

M_S	0
8	
7	
6	
5	
4	
3	
2	
1	
$M_L 0$	
-1	
-2	
-3	
-4	
-5	
-6	
-7	
-8	
	34

L=8 S=0, 2S+1=1, Microstates=34, Term= 1L (2-Terms)

M_S	+1	0	-1
7			
6			
5			
4			
3			
2			
1			
$M_L 0$			
-1			
-2			
-3			
-4			
-5			
-6			
-7			
	30	30	30

L=7, S=1, 2S+1=3, Microstates=90, Term= 3K (2-Terms)

M_S	0
7	
6	
5	
4	
3	
2	
1	
$M_L 0$	
-1	
-2	
-3	
-4	
-5	
-6	
-7	
	15

L=7, S=0, 2S+1=1, Microstates=15, Term= 1K

M_S	+2	+1	+0	-1	-2
6					
5					
4					
3					
2					
1					
$M_L 0$					
-1					
-2					
-3					
-4					
-5					
-6					
	13	13	13	13	13

L=6, S=2, 2S+1=5, Microstates=65, Term= 5I

M_S	+1	+0	-1
6			
5			
4			
3			
2			
1			
$M_L 0$			
-1			
-2			
-3			
-4			
-5			
-6			
	26	26	26

L=6, S=1, 2S+1=3, Microstates=78, Term= 3I (2-Terms)

M_S	+0
6	
5	
4	
3	
2	
1	
$M_L 0$	
-1	
-2	
-3	
-4	
-5	
-6	
39	

L=6, S=0, 2S+1=1, Microstates=39, Term=¹I (3-Terms)

M_S	+1	0	-1
5			
4			
3			
2			
1			
$M_L 0$			
-1			
-2			
-3			
-4			
-5			
	44	44	44

L=5, S=1, 2S+1=3, Microstates=132, Term=³H (4-Terms)

M_S	0
5	
4	
3	
2	
1	
$M_L 0$	
-1	
-2	
-3	
-4	
-5	
22	

L=5, S=0, 2S+1=1, Microstates=22, Term=¹H (2-Terms)

M_S	+2	+1	0	-1	-2
4					
3					
2					
1					
$M_L 0$					
-1					
-2					
-3					
-4					
	9	9	9	9	9

L=4, S=2, 2S+1=5, Microstates=45, Term=⁵G

M_S	+1	0	-1
4			
3			
2			
1			
$M_L 0$			
-1			
-2			
-3			
-4			
	27	27	27

L=4, S=1, 2S+1=3, Microstates=81, Term=³G (3-Terms)

M_S	+1
4	
3	
2	
1	
$M_L 0$	
-1	
-2	
-3	
-4	
36	

L=4, S=0, 2S+1=1, Microstates=36, Term=¹G (4-Terms)

M_S	+2	+1	0	-1	-2
3					
2					
1					
$M_L 0$					
-1					
-2					
-3					
	7	7	7	7	7

L=3, S=2, 2S+1=5, Microstates=35, Term=⁵F

M_S	+1	0	-1
3			
2			
1			
$M_L 0$			
-1			
-2			
-3			
	28	28	28

L=3, S=1, 2S+1=3, Microstates=84, Term=³F (4-Terms)

M_S	0
3	
2	
1	
$M_L 0$	
-1	
-2	
-3	
7	

L=3, S=0, 2S+1=1, Microstates=7, Term=¹F

M_S	+2	+1	0	-1	-2
2					
1					
M_L 0					
-1					
-2					
	5	5	5	5	5

$L=2, S=2, 2S+1=5, \text{Microstates}=25, \text{Term}={}^5D$

M_S	+1	0	-1
2			
1			
M_L 0			
-1			
-2			
	10	10	10

$L=2, S=1, 2S+1=3, \text{Microstates}=30, \text{Term}={}^3D$ (2-Terms)

M_S	0
M_L 0	
	2

$L=0, S=0, 2S+1=1, \text{Microstates}=2, \text{Term}={}^1S$ (2-Terms)

M_S	0
2	
1	
M_L 0	
-1	
-2	
	20

$L=2, S=0, 2S+1=1, \text{Microstates}=20, \text{Term}={}^1D$ (4-Terms)

M_S	+1	0	-1
1			
M_L 0			
-1			
	9	9	9

$L=1, S=1, 2S+1=3, \text{Microstates}=27, \text{Term}={}^3P$ (3-Terms)

M_S	+2	+1	0	-1	-2
M_L 0					
	1	1	1	1	1

$L=0, S=2, 2S+1=5, \text{Microstates}=5, \text{Term}={}^5S$

СРАВНИТЕЛНИ ИЗСЛЕДВАНИЯ НА АТОМНИТЕ ТЕРМОВИ СИМВОЛИ (ТЕРМОВЕ) НА RUSSELL-SAUNDERS ЗА ЕЛЕКТРОНИ ОТ nf^4 И nf^{10} -КОНФИГУРАЦИИ

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(Резюме)

Съществуват две спрегнати схеми за определянето на атомните термови символи (термове) на Russell-Saunders за еквивалентните електрони – схемата Russell-Saunders (L-S) и спин-орбиталната (j-j) схема. Атомните термови символи по Russell-Saunders дават информация за спектралните и магнитните свойства на атомите. В тази работа за извършени изчисления на всички възможни микро-състояния и атомни термове за електронните конфигурации nf^4 и nf^{10} , както и между атомните термове на Russell-Saunders на nf^4 и nf^{10} конфигурации. Възможните микро-състояния за тези конфигурации са 1001, а получените термове за тези състояния са 47, като тези термове са квинтети (5), триплети (22) и синглети (20). Термът на предсказаното основно състояние за двете конфигурации е квинтет I (5I). Основните състояния на nf^4 и nf^{10} конфигурациите са съответно 5I_4 и 5I_8 .