

j-j COUPLED ATOMIC TERMS FOR NONEQUIVALENT ELECTRONS OF $(n-1)f^x nd^1$ CONFIGURATIONS AND CORRELATION WITH L-S TERMS

P. L. Meena

University of Rajasthan (India)

Abstract. In this article j-j coupled atomic terms for $(n-1)f^x nd^1$ ($x=1$ and 3) configurations using microstate building method were computed and the j-j terms for $(n-1)f^1 nd^1$ configuration correlated pictorially with the L-S terms. The j-j coupled atomic terms derived for $(n-1)f^1 nd^1$ configuration are $[(7/2, 5/2) \text{ or } (f_{7/2})^1 (d_{5/2})^1]$, $[(7/2, 3/2) \text{ or } (f_{7/2})^1 (d_{3/2})^1]$, $[(5/2, 5/2) \text{ or } (f_{5/2})^1 (d_{5/2})^1]$ and $[(5/2, 3/2) \text{ or } (f_{5/2})^1 (d_{3/2})^1]$, and for $(n-1)f^3 nd^1$ configuration are $[(7/2, 7/2, 7/2, 5/2) \text{ or } (f_{7/2})^3 (d_{5/2})^1]$, $[(7/2, 7/2, 7/2, 3/2) \text{ or } (f_{7/2})^3 (d_{3/2})^1]$, $[(7/2, 7/2, 5/2, 5/2) \text{ or } (f_{7/2})^2 (f_{5/2})^1 (d_{5/2})^1]$, $[(7/2, 7/2, 5/2, 3/2) \text{ or } (f_{7/2})^2 (f_{5/2})^1 (d_{3/2})^1]$, $[(7/2, 5/2, 5/2, 5/2) \text{ or } (f_{7/2})^1 (f_{5/2})^2 (d_{5/2})^1]$, $[(7/2, 5/2, 5/2, 3/2) \text{ or } (f_{7/2})^1 (f_{5/2})^2 (d_{3/2})^1]$, $[(5/2, 5/2, 5/2, 5/2) \text{ or } (f_{5/2})^3 (d_{5/2})^1]$ and $[(5/2, 5/2, 5/2, 3/2) \text{ or } (f_{5/2})^3 (d_{3/2})^1]$.

Keywords: angular momentum; jj coupling; j-j coupled term; L-S coupling; microstate

Introduction

Obtaining of the atomic terms and states from a given atomic configuration is by now a conventional topic in inorganic chemistry (Li et al., 2008; Atkins et al., 2006; Hoescroff & Sharpe, 2008). Atomic terms derived by coupling angular momentum that described by two schemes one is L-S and another is j-j scheme. In the L-S coupling scheme, it is assumed that electronic repulsion is much greater than spin-orbit interaction and it is appropriate where, the inter-electronic repulsion is much larger than the spin orbit interaction. Number of methods have been developed to derive the L-S terms for electronic configuration via Partitioning technique (Olson, 2011), Partial term method (Kiremire, 1990), Partitioning total spin method (Chen, 1989), Group representation method (Guofan & Ellzey, 1987), Numerical algorithm method (Kiremire, 1987), Spin factoring method (McDaniel, 1977), Hyde method (Hyde, 1975), Ford method (Ford, 1972), Group theoretical method (Judd, 1967; Wybourne, 1966), Generating functions derived via group theory method (Curl & Kilpatrick, 1960), Slater graphics (Slater, 1960), Quantum

mechanical method (Russell & Saunders, 1925), Vector model (Landé, 1921) and Microstate building method by electronic arrangement (Meena et al., 2012; Meena et al., 2013).

j-j coupling becomes more significant than the L-S coupling in heavy atoms and L-S coupling gradually change to j-j coupling in going from light to heavy atom. j-j coupled atomic terms can be obtained by different ways such as electronic arrangement (Meena et al., 2015); Orofino & Faria, 2010; Novak, 1999; Campbell, 1998; Gauerke & Campbell, 1994; Haigh, 1995; Rubio & Perez, 1986; Richtmyer et al., 1969; Tuttle, 1967). The j-j coupling scheme becomes more treatable in chemistry when the microstates are built by arranging electrons and this makes easy to get the terms also. The notations for L-S terms are universally standardized but not for the j-j coupling terms. The common notation systems for the j-j coupling terms that are designated by the j's as $[(j_1, j_2, \dots)_I]$ (Haigh, 1995) and $[(j_1)^a(j_2)^b(j_3)^c \dots]$ (Rubio & Perez, 1986; Richtmyer et al., 1969; Tuttle, 1967) but in some systems the terms are designated by l's as $[(l_{\ell-1/2})^a(l_{\ell+1/2})^b(l'_{\ell'-1/2})^c \dots]$ (Gauerke & Campbell, 1994) where l and l' are letter designations for orbital's, and ℓ and ℓ' are the numerical values of the angular momentum quantum numbers for the electrons. In this article I used both $(j_1, j_2, j_3)_I$ and $[(l_{\ell-1/2})^a(l_{\ell+1/2})^b(l'_{\ell'-1/2})^c \dots]$ notations to represent the j-j coupled atomic terms.

Methodology

Number of microstates for electrons of $(n-1)f^x nd^1$ ($n=1\&3$) configuration

Total number of microstates for any electronic configuration is given by an expression, $N = \frac{n!}{x(n-x)!}$ Where $n = 2(2l+1)$ and x = total number of electrons in sub shell.

$$\begin{aligned} \text{For } (n-1)f^1 nd^1 \text{ configuration, } n=14 \& 10 \text{ and } x=1\&1, N &= \frac{14!}{1!(14-1)!} x \\ \frac{10!}{1!(10-1)!} &= 140, \text{ and for } (n-1)f^3 nd^1 \text{ configuration, } n=14 \& 10 \text{ and } x=3\&1, N= \\ \frac{14!}{3!(14-3)!} \times \frac{10!}{1!(10-1)!} &= 3640 \end{aligned}$$

Number of terms for $(n-1)f^x nd^1$ ($x=1\&3$) configuration

Number of terms for a particular electronic state with equivalent electrons are $(x+1)$, for subshell less than half filled, 'x' for half filled subshell, and $(4\ell+3-x)$ for subshell more than half filled, where 'x' represent total number of electrons in partially filled subshell and ' ℓ ' is numerical value of the angular momentum quantum numbers for electrons (Gauerke & Campbell, 1994). But for the electronic state with nonequivalent electrons $[(n-1)f^x nd^1]$ the number of terms are $[(x+1)(y+1)]$. In

$(n-1)f^x nd^1$ ($x=1\&3$) configurations total j-j terms are four and eight. The possible j values for f electrons are $j=7/2$ or $5/2$ and for d electron $5/2$ or $3/2$, and the j-j terms ($j_1, j_2, \dots$) derived for $(n-1)f^1 nd^1$ configuration are $(7/2, 5/2)$, $(7/2, 3/2)$, $(5/2, 5/2)$ and $(5/2, 3/2)$, and for $(n-1)f^3 nd^1$ configuration the terms are $(7/2, 7/2, 7/2, 5/2)$, $(7/2, 7/2, 7/2, 3/2)$, $(7/2, 7/2, 5/2, 5/2)$, $(7/2, 7/2, 5/2, 3/2)$, $(7/2, 5/2, 5/2, 5/2)$, $(7/2, 5/2, 5/2, 3/2)$, $(5/2, 5/2, 5/2, 5/2)$ and $(5/2, 5/2, 5/2, 3/2)$. j-j terms in the form of $[(l_{t-1/2})^i (l_{t+1/2})^{n-i}]$ notation will be $[(f_{7/2})^1 (d_{5/2})^1]$, $[(f_{7/2})^1 (d_{3/2})^1]$, $[(f_{5/2})^1 (d_{5/2})^1]$ and $[(f_{5/2})^1 (d_{3/2})^1]$ for $(n-1)f^1 nd^1$ configuration and $[(f_{7/2})^3 (d_{5/2})^1]$, $[(f_{7/2})^3 (d_{3/2})^1]$, $[(f_{7/2})^2 (f_{5/2})^1 (d_{5/2})^1]$, $[(f_{7/2})^2 (f_{5/2})^1 (d_{3/2})^1]$, $[(f_{7/2})^1 (f_{5/2})^2 (d_{5/2})^1]$, $[(f_{7/2})^1 (f_{5/2})^2 (d_{3/2})^1]$, $[(f_{5/2})^3 (d_{5/2})^1]$ and $[(f_{5/2})^3 (d_{3/2})^1]$ for $(n-1)f^3 nd^1$ configuration.

Number of microstates for particular j-j atomic term

Number of microstates for a particular j-j term of the form $[(l_{t-1/2})^i (l_{t+1/2})^{n-i}]$ or (j_1, j_2, j_3, j_4) for each sub set of equivalent electrons is given by

$$\frac{(2\ell)!(2\ell+2)!}{i!(2\ell-i)!(n-i)!(2\ell+2+i-n)!} \text{ and for nonequivalent electrons it is given by } \frac{(2\ell)!(2\ell+2)!}{i!(2\ell-i)!(n-i)!(2\ell+2+i-n)!} x \frac{(2\ell)!(2\ell+2)!}{i!(2\ell-i)!(n-i)!(2\ell+2+i-n)!}$$

For the term $(7/2, 5/2)$ or $[(f_{7/2})^1 (d_{5/2})^1]$ of $(n-1)f^1 nd^1$ configuration total microstates will be

$$\frac{(2x3)!(2x3+2)!}{0!(2x3-0)!(1-0)!(2x3+2+0-1)!} x \frac{(2x2)!(2x2+2)!}{0!(2x2-0)!(1-0)!(2x2+2+0-1)!} = 48$$

And for the term $(7/2, 7/2, 7/2, 5/2)$ or $[(f_{7/2})^3 (d_{5/2})^1]$ of $(n-1)f^3 nd^1$ configuration total microstates will be

$$\frac{(2x3)!(2x3+2)!}{0!(2x3-0)!(3-0)!(2x3+2+0-3)!} x \frac{(2x2)!(2x2+2)!}{0!(2x2-0)!(1-0)!(2x2+2+0-1)!} = 336$$

Computed microstates for j-j coupled atomic terms of $(n-1)f^x nd^1$ ($n=1\&3$) configurations are given in Tables 1 and 2.

Table 1. Total microstates for j-j coupled terms of $(n-1)f^1 nd^1$ configuration

E1 j_1	E2 j_2	jj coupled terms	MS	MJ values
7/2	5/2	$(7/2, 5/2)$ or $[(f_{7/2})^1 (d_{5/2})^1]$	48	-6 to +6
7/2	3/2	$(7/2, 3/2)$ or $[(f_{7/2})^1 (d_{3/2})^1]$	32	-5 to +5
5/2	5/2	$(5/2, 5/2)$ or $[(f_{5/2})^1 (d_{5/2})^1]$	36	-5 to +5
5/2	3/2	$(5/2, 3/2)$ or $[(f_{5/2})^1 (d_{3/2})^1]$	24	-4 to +4

*E1 and E2 represent electrons and MS is Microstate

Table 2. Total of microstates for j-j coupled terms of (n-1)f³ nd¹ configuration

E1 _{j₁}	E2 _{j₂}	E3 _{j₃}	E4 _{j₄}	jj coupled terms	MS	MJ values
7/2	7/2	7/2	5/2	(7/2, 7/2, 7/2, 5/2) or [(f _{7/2}) ³ (d _{5/2}) ¹]	336	-10 to +10
7/2	7/2	7/2	3/2	(7/2, 7/2, 7/2, 3/2) or [(f _{7/2}) ³ (d _{3/2}) ¹]	224	-9 to +9
7/2	7/2	5/2	5/2	(7/2, 7/2, 5/2, 5/2) or [(f _{7/2}) ² (f _{5/2}) ¹ (d _{5/2}) ¹]	1008	-11 to +11
7/2	7/2	5/2	3/2	(7/2, 7/2, 5/2, 3/2) or [(f _{7/2}) ² (f _{5/2}) ¹ (d _{3/2}) ¹]	672	-10 to +10
7/2	5/2	5/2	5/2	(7/2, 5/2, 5/2, 5/2) or [(f _{7/2}) ¹ (f _{5/2}) ² (d _{5/2}) ¹]	720	-10 to +10
7/2	5/2	5/2	3/2	(7/2, 5/2, 5/2, 3/2) or [(f _{7/2}) ¹ (f _{5/2}) ² (d _{3/2}) ¹]	480	-9 to +9
5/2	5/2	5/2	5/2	(5/2, 5/2, 5/2, 5/2) or [(f _{5/2}) ³ (d _{5/2}) ¹]	120	-7 to +7
5/2	5/2	5/2	3/2	(5/2, 5/2, 5/2, 3/2) or [(f _{5/2}) ³ (d _{3/2}) ¹]	80	-6 to +6

*E1, E2, E3 and E4 represent electrons and MS is Microstate

Table 3. Removal of microstates for J levels in (7/2, 5/2) j-j coupled term for (n-1)f¹ nd¹ configuration

M _j	Total MS	MS after removing J=6 level	MS after removing J=5 level	MS after removing J=4 level	MS after removing J=3 level	MS after removing J=2 level
6	1	-	-	-	-	-
5	2	1	-	-	-	-
4	3	2	1	-	-	-
3	4	3	2	1	-	-
2	5	4	3	2	1	-
1	6	5	4	3	2	1
0	6	5	4	3	2	1

J levels for j-j coupled electronic terms for (n-1)f¹ nd¹ configuration

J levels for j-j coupled terms are obtained by eliminating the microstates associated with the particular J level from microstate tables starting from maximum M_j value and further moving to the lowest J level. From the Table 3 for the j-j coupled term (7/2, 5/2) or [(f_{7/2})¹ (d_{5/2})¹] for (n-1)f¹ nd¹ configuration the maximum M_j values is 6 which results into J=6 level for this term, when the 13 microstates associated with J= 6 level are eliminated, and the next maximum M_j obtained is 5 that yield another J level by elimination of 11 microstates associated with this J=5 level, and further elimination of 9, 7, 5 and 3 microstates produce 4, 3, 2 and 1 J levels for this term. The same procedure is applied for other j-j coupled terms for (n-1)f¹ nd¹ configuration as illustrated in Table 4 for (7/2, 3/2) or [(f_{7/2})¹ (d_{3/2})¹] term, in Table 5 for (5/2, 5/2) or [(f_{5/2})¹ (d_{5/2})¹] term, in Table 6 for (5/2, 3/2) or [(f_{5/2})¹ (d_{3/2})¹] term.

Table 4. Removal of microstates for J levels in (7/2, 3/2) j-j coupled term for (n-1)f¹ nd¹ configuration

M _J	Total MS	MS after removing J=5 level	MS after removing J=4 level	MS after removing J=3 level	MS after removing J=2 level
5	1	-	-	-	-
4	2	1	-	-	-
3	3	2	1	-	-
2	4	3	2	1	-
1	5	4	3	2	1
0	5	4	3	2	1

Table 5. Removal of microstates for J levels in (5/2, 5/2) j-j coupled term for (n-1)f¹ nd¹ configuration

M _J	Total MS	MS after removing J=5 level	MS after removing J=4 level	MS after removing J=3 level	MS after removing J=2 level	MS after removing J=1 level
5	1	-	-	-	-	-
4	2	1	-	-	-	-
3	3	2	1	-	-	-
2	4	3	2	1	-	-
1	5	4	3	2	1	-
0	6	5	4	3	2	1

Table 6. Removal of microstates for J levels in (5/2, 3/2) j-j coupled term for (n-1)f¹ nd¹ configuration

M _J	Total MS	MS after removing J=4 level	MS after removing J=3 level	MS after removing J=2 level
4	1	-	-	-
3	2	1	-	-
2	3	2	1	-
1	4	3	2	1
0	4	3	2	1

J levels for j-j coupled atomic terms for (n-1)f³ nd¹ configuration

For j-j coupled term (7/2, 7/2, 7/2, 5/2) or [(f_{7/2})³ (d_{5/2})¹] of (n-1)f³ nd¹ configuration the maximum M_J values is 10 which results into J=10 level for this term, when the 21 microstates associated with J=10 level are eliminated, and the next maxi-

num M_J obtained is 9 that yield another J level by elimination of 19 microstates associated with this J=9 level, and further elimination of 34, 45, 52, 55, 45, 35, 20, 9 and 1 microstates produce 8(2), 7(3), 6(4), 5(5), 4(5), 3(5), 2(4), 1(3) and 0 J levels for this term as shown in Table 7.

Table 7. Removal of microstates for J levels in (7/2, 7/2, 7/2, 5/2) j-j coupled term for $(n-1)f^3 nd^1$ configuration

M_J	Total MS	MS after J=10 level	MS after J=9 level	MS after J=8 levels	MS after J=7 levels	MS after J=6 levels	MS after J=5 levels	MS after J=4 levels	MS after J=3 levels	MS after J=2 levels	MS after J=1 levels
10	1	-	-	-	-	-	-	-	-	-	-
9	2	1	-	-	-	-	-	-	-	-	-
8	4	3	2	-	-	-	-	-	-	-	-
7	7	6	5	3	-	-	-	-	-	-	-
6	11	10	9	7	4	-	-	-	-	-	-
5	16	15	14	12	9	5	-	-	-	-	-
4	21	20	19	17	14	10	5	-	-	-	-
3	26	25	24	22	19	15	10	5	-	-	-
2	30	29	28	26	23	19	14	9	4	-	-
1	33	32	31	29	26	22	17	12	7	3	-
0	34	33	32	30	27	23	18	13	8	4	1
-1	33	32	31	29	26	22	17	12	7	3	-
-2	30	29	28	26	23	19	14	9	4	-	-
-3	26	25	24	22	19	15	10	5	-	-	-
-4	21	20	19	17	14	10	5	-	-	-	-
-5	16	15	14	12	9	5	-	-	-	-	-
-6	11	10	9	7	4	-	-	-	-	-	-
-7	7	6	5	3	-	-	-	-	-	-	-
-8	4	3	2	-	-	-	-	-	-	-	-
-9	2	1	-	-	-	-	-	-	-	-	-
-10	1	-	-	-	-	-	-	-	-	-	-
Total	336	315	296	262	217	165	110	65	30	10	1

The same procedure is applied for other j-j coupled terms for $(n-1)f^3 nd^1$ configuration as illustrated in Table 8 for (7/2, 7/2, 7/2, 3/2) or $[(f_{7/2})^3 (d_{3/2})^1]$ term, in Table

9 for $(7/2, 7/2, 5/2, 5/2)$ or $[(f_{7/2})^2(f_{5/2})^1(d_{5/2})^1]$ term, in Table 10 for $(7/2, 7/2, 5/2, 3/2)$ or $[(f_{7/2})^2(f_{5/2})^1(d_{3/2})^1]$ term, in Table 11 for $(7/2, 5/2, 5/2, 5/2)$ or $[(f_{7/2})^1(f_{5/2})^2(d_{5/2})^1]$ term, in Table 12 for $(7/2, 5/2, 5/2, 3/2)$ or $[(f_{7/2})^1(f_{5/2})^2(d_{3/2})^1]$ term, in Table 13 for $(5/2, 5/2, 5/2, 5/2)$ or $[(f_{5/2})^3(d_{5/2})^1]$ term and in Table 14 for $(5/2, 5/2, 5/2, 3/2)$ or $[(f_{5/2})^3(d_{3/2})^1]$ term.

Table 8. Removal of microstates for J levels in $(7/2, 7/2, 7/2, 3/2)$ j-j coupled term for $(n-1)f^8 nd^1$ configuration

M_J	Total MS	MS after J=9 level	MS after J=8 level	MS after J=7 levels	MS after J=6 levels	MS after J=5 levels	MS after J=4 levels	MS after J=3 levels	MS after J=2 levels	MS after J=1 levels
9	1	-	-	-	-	-	-	-	-	-
8	2	1	-	-	-	-	-	-	-	-
7	4	3	2	-	-	-	-	-	-	-
6	7	6	5	3	-	-	-	-	-	-
5	10	9	8	6	3	-	-	-	-	-
4	14	13	12	10	7	4	-	-	-	-
3	18	17	16	14	11	8	4	-	-	-
2	21	20	19	17	14	11	7	3	-	-
1	23	22	21	19	16	13	9	5	2	-
0	24	23	22	20	17	14	10	6	3	1

Table 9. Removal of microstates for J levels in $(7/2, 7/2, 5/2, 5/2)$ j-j coupled term for $(n-1)f^8 nd^1$ configuration

M_J	Total MS	MS after J=11 level	MS after J=10 levels	MS after J=9 level	MS after J=8 levels	MS after J=7 levels	MS after J=6 levels	MS after J=5 levels	MS after J=4 levels	MS after J=3 levels	MS after J=2 levels	MS after J=1 levels
11	1	-	-	-	-	-	-	-	-	-	-	-
10	3	2	-	-	-	-	-	-	-	-	-	-
9	7	6	4	-	-	-	-	-	-	-	-	-
8	13	12	10	6	-	-	-	-	-	-	-	-
7	22	21	19	15	9	-	-	-	-	-	-	-
6	34	33	31	27	21	12	-	-	-	-	-	-
5	48	47	45	41	35	26	14	-	-	-	-	-

4	63	62	60	56	50	41	29	15	-	-	-	-
3	77	76	74	70	64	55	43	29	14	-	-	-
2	89	88	86	82	76	67	55	41	26	12	-	-
1	97	96	94	90	84	75	63	49	34	20	8	-
0	100	99	97	93	87	78	66	52	37	23	11	3

Table 10. Removal of microstates for J levels in (7/2, 7/2, 5/2, 3/2) j-j coupled term for (n-1)f³ nd¹ configuration

M _J	Total MS	MS after J=10 level	MS after J=9 levels	MS after J=8 levels	MS after J=7 levels	MS after J=6 levels	MS after J=5 levels	MS after J=4 levels	MS after J=3 levels	MS after J=2 levels	MS after J=1 levels
10	1	-	-	-	-	-	-	-	-	-	-
9	3	2	-	-	-	-	-	-	-	-	-
8	6	5	3	-	--	-	-	-	-	-	-
7	13	12	10	7	-	-	-	-	-	-	-
6	21	20	18	15	8	-	-	-	-	-	-
5	31	30	28	25	18	10	-	-	-	-	-
4	42	41	39	36	29	21	11	-	-	-	-
3	53	52	50	47	40	32	22	11	-	-	-
2	63	62	60	57	50	42	32	21	10	-	-
1	68	67	65	62	55	47	37	26	15	5	-
0	70	69	67	64	57	49	39	28	17	7	2

Table 11. Removal of microstates for J levels in (7/2, 5/2, 5/2, 5/2) j-j coupled term for (n-1)f³ nd¹ configuration

M _J	Total MS	MS after J=10 level	MS after J=9 levels	MS after J=8 levels	MS after J=7 levels	MS after J=6 levels	MS after J=5 levels	MS after J=4 levels	MS after J=3 levels	MS after J=2 levels	MS after J=1 levels
10	1	-	-	-	-	-	-	-	-	-	-
9	3	2	-	-	-	-	-	-	-	-	-
8	7	6	4	-	-	-	-	-	-	-	-
7	13	12	10	6	-	-	-	-	-	-	-
6	22	21	19	15	9	-	-	-	-	-	-
5	33	32	30	26	20	11	-	-	-	-	-
4	45	44	42	38	32	23	12	-	-	-	-
3	57	56	54	50	44	35	24	12	-	-	-

2	67	66	64	60	54	45	34	22	10	-	-
1	74	73	71	67	61	52	41	29	17	7	-
0	76	75	73	69	63	54	43	31	19	9	2

Table 12. Removal of microstates for J levels in (7/2, 5/2, 5/2, 3/2) j-j coupled term for (n-1)f³ nd¹ configuration

M _J	Total MS	MS after J=9 level	MS after J=8 levels	MS after J=7 levels	MS. After J=6 levels	MS after J=5 levels	MS after J=4 levels	MS after J=3 levels	MS after J=2 levels	MS after J=1 levels
9	1	-	-	-	-	-	-	-	-	-
8	3	2	-	-	-	-	-	-	-	-
7	7	6	4	-	-	-	-	-	-	-
6	13	12	10	6	-	-	-	-	-	-
5	21	20	18	14	8	-	-	-	-	-
4	30	29	27	23	17	9	-	-	-	-
3	39	38	36	32	26	18	9	-	-	-
2	47	46	44	40	34	26	17	8	-	-
1	52	51	49	45	39	31	22	13	5	-
0	54	53	51	47	41	33	24	15	7	2

Table 13. Removal of microstates for J levels in (5/2, 5/2, 5/2, 5/2) j-j coupled term for (n-1)f³ nd¹ configuration

M _J	Total MS	MS after J=7 level	MS after J=6 level	MS after J=5 levels	MS after J=4 levels	MS after J=3 levels	MS after J=2 levels	MS after J=1 levels
7	1	-	-	-	-	-	-	-
6	2	1	-	-	-	-	-	-
5	4	3	2	-	-	-	-	-
4	7	6	5	3	-	-	-	-
3	10	9	8	6	3	-	-	-
2	13	12	11	9	6	3	-	-
1	15	14	13	11	8	5	2	-
0	16	15	14	12	9	6	3	1

Table 14. Removal of microstates for J levels in (5/2, 5/2, 5/2, 3/2) j-j coupled term for (n-1)f³nd¹ configuration

M _J	Total MS	MS after J=6 level	MS after J=5 levels	MS after J=4 levels	MS after J=3 levels	MS after J=2 levels	MS after J=1 levels
6	1	-	-	-	-	-	-
5	2	1	-	-	-	-	-
4	4	3	2	-	-	-	-
3	7	6	5	3	-	-	-
2	9	8	7	5	2	-	-
1	11	10	9	7	4	2	-
0	12	11	10	8	5	3	1

Results and discussion

For (n-1)f¹nd¹ configuration four j-j coupled atomic terms derived which are [{(7/2, 5/2) or (f_{7/2})¹(d_{5/2})¹}_{6, 5, 4, 3, 2, 1}], [{(7/2, 3/2) or (f_{7/2})¹(d_{3/2})¹}_{5, 4, 3, 2}], [{(5/2, 5/2) or (f_{5/2})¹(d_{5/2})¹}_{5, 4, 3, 2, 1, 0}] and [{(5/2, 3/2) or (f_{5/2})¹(d_{3/2})¹}_{4, 3, 2, 1}], and for the (n-1)f³nd¹ configuration eight j-j terms derived which are [{(7/2, 7/2, 7/2, 5/2) or (f_{7/2})³(d_{5/2})¹}_{10, 9, 8(2), 7(3), 6(4), 5(5), 4(5), 3(5), 2(4), 1(3), 0}], [{(7/2, 7/2, 7/2, 3/2) or (f_{7/2})³(d_{3/2})¹}_{9, 8, 7(2), 6(3), 5(3), 4(4), 3(4), 2(3), 1(2), 0}], [{(7/2, 7/2, 5/2, 5/2) or (f_{7/2})²(f_{5/2})¹(d_{5/2})¹}_{11, 10(2), 9(4), 8(6), 7(9), 6(12), 5(14), 4(15), 3(14), 2(12), 1(8), 0(3)}], [{(7/2, 7/2, 5/2, 3/2) or (f_{7/2})²(f_{5/2})¹(d_{3/2})¹}_{10, 9(2), 8(3), 7(7), 6(8), 5(10), 4(11), 3(11), 2(10), 1(5), 0(2)}], [{(7/2, 5/2, 5/2, 5/2) or (f_{7/2})¹(f_{5/2})²(d_{5/2})¹}_{10, 9(2), 8(4), 7(6), 6(9), 5(11), 4(12), 3(12), 2(10), 1(7), 0(2)}], [{(7/2, 5/2, 5/2, 3/2) or (f_{7/2})¹(f_{5/2})²(d_{3/2})¹}_{9, 8(2), 7(4), 6(6), 5(8), 4(9), 3(9), 2(8), 1(5), 0(2)}], [{(5/2, 5/2, 5/2, 5/2) or (f_{5/2})³(d_{5/2})¹}_{7, 6, 5(2), 4(3), 3(3), 2(3), 1(2), 0}] and [{(5/2, 5/2, 5/2, 3/2) or (f_{5/2})³(d_{3/2})¹}_{6, 5, 4(2), 3(3), 2(2), 1(2), 0}].

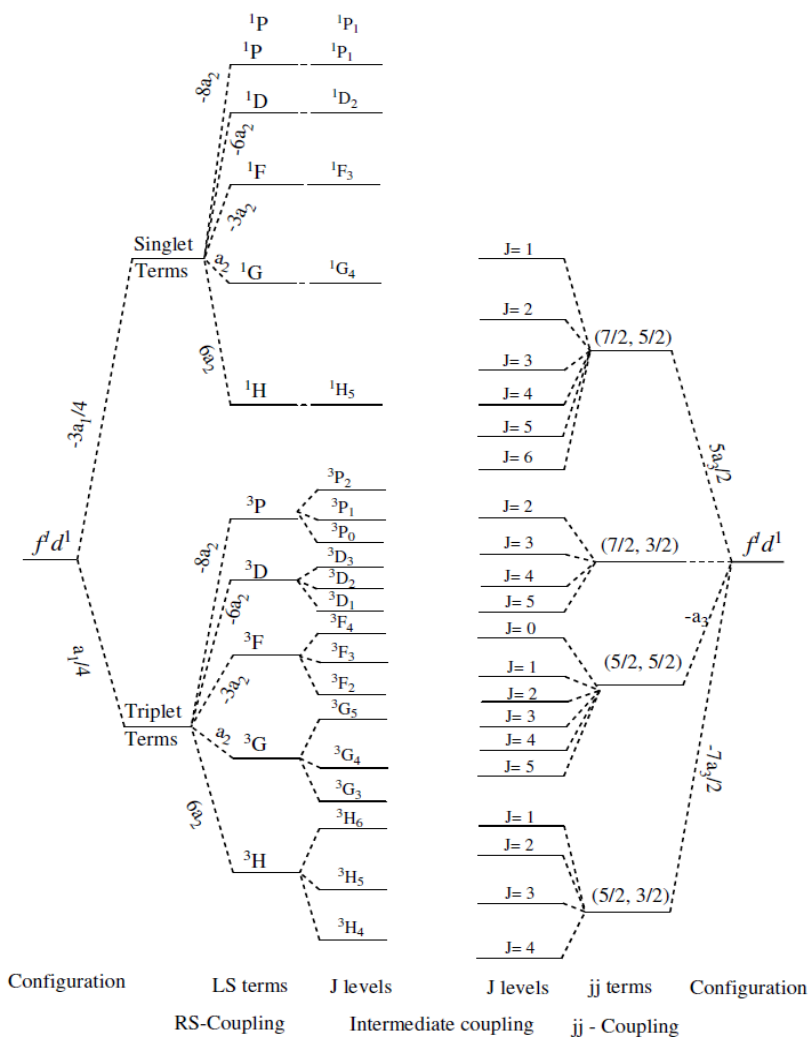


Figure 1. Pictorially correlation of L-S and j-j atomic terms & electronic states for the $(n-1)f^1 nd^1$ configuration

Conclusion

In this article I have derived j-j coupled atomic terms and electronic states (J-levels) for nonequivalent electrons of $(n-1)f^x nd^1$ ($x=1 \text{ \& } 3$) configurations using simple method and the j-j terms and electronic states for $(n-1)f^1 nd^1$ configuration

correlated pictorially with L-S terms as shown in Fig. 1.

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✉ **Dr. P. L. Meena**

Department of Chemistry
University of Rajasthan

Jaipur, Rajasthan-302004, India

E-mail: parmeshwar1978@gmail.com