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

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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) or $(f_{7/2})^1 (d_{5/2})^1$], [(7/2, 3/2) or $(f_{7/2})^1 (d_{3/2})^1$], [(5/2, 5/2) or $(f_{5/2})^1 (d_{5/2})^1$] and [(5/2, 3/2) 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) or $(f_{7/2})^3 (d_{5/2})^1$], [(7/2, 7/2, 7/2, 3/2) or $(f_{7/2})^3 (d_{3/2})^1$], [(7/2, 7/2, 5/2, 5/2) or $(f_{7/2})^2 (f_{5/2})^1 (d_{5/2})^1$], [(7/2, 7/2, 5/2, 3/2) or $(f_{7/2})^2 (f_{5/2})^1 (d_{3/2})^1$], [(7/2, 5/2, 5/2, 5/2) or $(f_{7/2})^1 (f_{5/2})^2 (d_{5/2})^1$], [(7/2, 5/2, 5/2, 3/2) or $(f_{7/2})^1 (f_{5/2})^2 (d_{3/2})^1$], [(5/2, 5/2, 5/2, 5/2) or $(f_{5/2})^3 (d_{5/2})^1$] and [(5/2, 5/2, 5/2, 3/2) 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 $[(j_1, j_2....)_J]$ (Haigh, 1995) and $[(j_1)^a(j_2)^b(j_3)^c...]$ (Rubio & Perez, 1986; Richtmyer et al., 1969; Tuttle, 1967) but in some systems the terms are designated by *l*'s as $[(l_{\ell-1/2})^a\ (l_{\ell+1/2})^b\ (l'_{\ell'-1/2})^c...]$ (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 $(j_1, j_2, j_3)_J$ and $[(l_{\ell-1/2})^a\ (l_{\ell+1/2})^b\ (l'_{\ell'-1/2})^c...]$ 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(2*l*+1) and x= total number of electrons in sub shell.

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

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 (4ℓ+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^y] 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 $(j_1, j_2\ldots)$ 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 $[(l_{\ell-1/2})^i\ (l_{\ell+1/2})^{n-i}]$ 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 $[(l_{\ell-1/2})^i\ (l_{\ell+1/2})^{n-i}]$ or (j_1, j_2, j_3, j_4) for each sub set of equivalent electrons is given by

$$\frac{(2\ell)!(2\ell+2)!}{i!(2\ell-i)!(n-i)!(2\ell+2+i-n)!}$$

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)f^3 nd^1 configuration

E1j_1	E2j_2	E3j_3	E4j_4	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)f^1 nd^1 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)f^1 nd^1 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)f^1 nd^1 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)f^1 nd^1 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 $(n\text{-}1)f^1\ nd^1$ configuration

M_J	Total MS	MS after removing J=5 level	MS after removing J=4 level	MS after removing J=3level	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 $(n\text{-}1)f^1\ nd^1$ 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 $(n\text{-}1)f^1\ nd^1$ 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 $(n\text{-}1)f^3\ nd^1$ configuration

For j-j coupled term (7/2, 7/2, 7/2, 5/2) or $[(f_{7/2})^3\ (d_{5/2})^1]$ of $(n\text{-}1)f^3\ nd^1$ 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 maximum 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 $(n\text{-}1)f^3\, nd^1$ 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 $(n\text{-}1)f^3\, nd^1$ 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)f^3 nd^1 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)f^3 nd^1 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)f^3 nd^1 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)f^3 nd^1 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)f^3 nd^1 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)f^1 nd^1 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) f^3 nd^1 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 $(f_{5/2})^3 (d_{3/2})^1\}_{6, 5, 4(2), 3(3), 2(2), 1(2), 0}$].

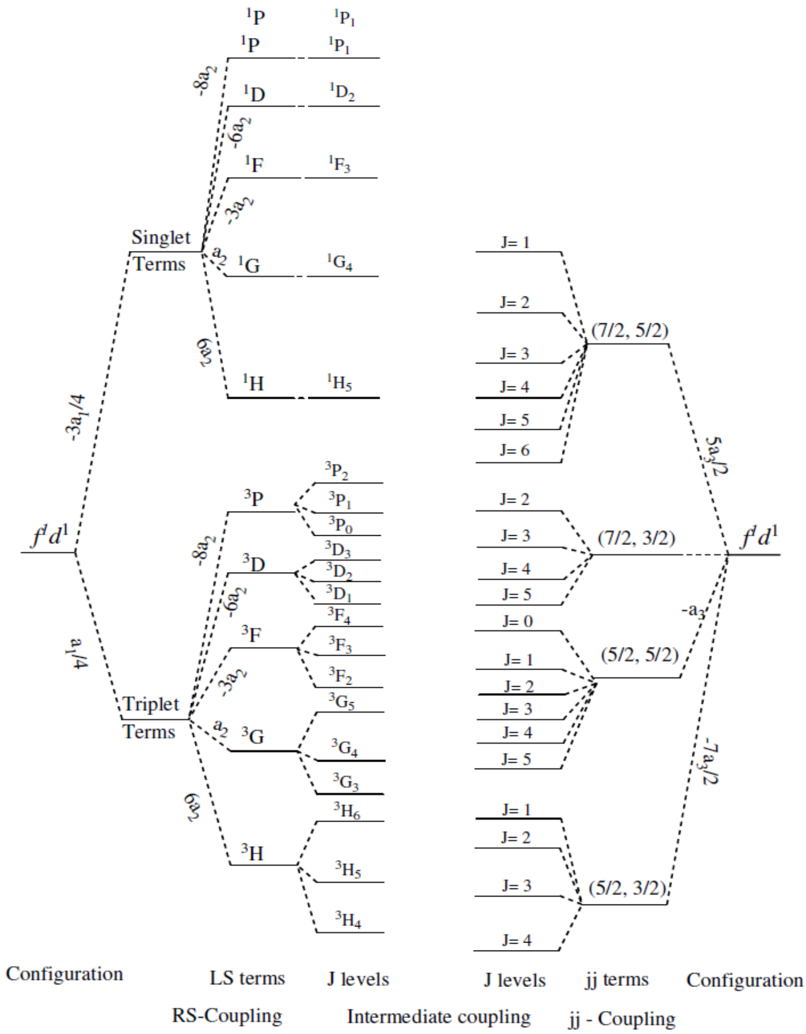

Figure 1. Pictorially correlation of L-S and j-j atomic terms & electronic states for the (n-1)f^1 nd^1 configuration

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 & 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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REFERENCES

Atkins, P., Overton, T., Rourke, J., Weller, M. & Armstrong, F. (2006). *Inorganic chemistry*. Oxford: Oxford University Press.

Campbell, M.L. (1998). Rules for determining the ground state of a j-j coupled atom. *J. Chem. Educ., 75,* 1339 – 1340.

Chen, J.-H. (1989). Atomic term symbols by group representation methods. *J. Chem. Educ., 66,* 893 – 897.

Curl, R.F. & Kilpatrick, J.E. (1960). Atomic term symbols by group theory. *Amer. J. Phys., 28,* 357 – 365.

Ford, D.I. (1972). Molecular term symbols by group theory. *J. Chem. Educ., 49,* 336 – 340.

Gauerke, E.S.J. & Campbell, M.L. (1994). A simple, systematic method for determining j levels for jj coupling. *J. Chem. Educ., 71,* 457 – 462.

Guofan, L. & Ellzey, M.L. (1987). Finding the terms of configurations of equivalent electrons by partitioning total spins. *J. Chem. Educ., 64,* 771 – 772.

Haigh, C.W. (1995). The theory of atomic spectroscopy: jj coupling, intermediate coupling, and configuration interaction. *J. Chem. Educ., 72,* 206 – 209.

Housecroft, C.E. & Sharpe, A.G. (2008). *Inorganic chemistry*. Essex: Pearson Education.

Hyde, K.E. (1975). Methods for obtaining Russell-Sounders term symbols from electronic configurations. *J. Chem. Educ., 52,* 87 – 89.

Judd, B.R. (1967). Atomic shell theory recast. *Phys. Rev., 162,* 28 – 37.

Kiremire, E.M.R. (1987). A numerical algorithm technique for deriving Russell-Sounders (R-S) terms. *J. Chem. Educ., 64,* 951 – 953.

Kiremire, E.M.R. (1990). Partial and ligand field terms. *J. Chem. Educ., 67,* 216 – 217.

Landé, A. (1921). Über den anomalen Zeeman effekt. *Z. Physik, 5,* 231 – 241.

Li, W.-K., Zhou, G.-D. & Mak, T. (2008). *Advanced structural inorganic chemistry*. Oxford: Oxford University Press.

McDaniel, D.H. (1977). Spin factoring as an aid in the determination of spectroscopic terms. *J. Chem. Educ., 54,* 147 – 149.

Meena, P.L., Meena, A.S., Meena, K.M. & Kumar, N. (2013). Atomic term symbols (terms) for nonequivalent electrons of (n-1)f^3 nd^1 configuration via Russell-Saunders coupling scheme. *Int. J. Chem., 34,* 1236 – 1242.

Meena, P.L., Kumar, N., Meena, K.S. & Jain, P.K. (2012). Calculation of atomic spectroscopic terms for non-equivalent electrons of f^2d^1 configuration and assigning the term symbols. *Asian J. Chem., 24,* 5677 – 5679.

Meena, P.L., Meena, A.S., Kumar, N. & Meena, K.S. (2015). Obtaining jj coupled spectroscopic terms for nonequivalent electrons of (n-1)f^2 nd^1 configuration. *Chem. Educator, 20,* 34 – 38.

Novak, I. (1999). When do arrows not have tips. *J. Chem. Educ., 76,* 1380 – 1381.

Olson, J.A. (2011). Atomic term symbols via partitioning techniques. *Int. J. Quantum Chem., 111,* 2844 – 2850.

Orofino, H. & Faria, R.B. (2010). Obtaining the electron angular momentum coupling spectroscopic terms, jj, *J. Chem. Educ., 87,* 1451 – 1454.

Richtmyer, K., Kennard, E.H. & Cooper, J.N. (1969). *Introduction to modern physics*. New York: McGraw- Hill.

Rubio, J. & Perez, J.J. (1986). Energy levels in the jj coupling scheme. *J. Chem. Educ., 63,* 476 – 478.

Russell, H.N. & Saunders, F.A. (1925). New regularities in the spectra of the alkaline earths. *Astrophys. J., 61,* 38 – 69.

Slater, J.C. (1960). *Quantum theory of atomic structure*. New York: McGraw-Hill.

Tuttle, E.R. (1967). Terms obtained from configurations of equivalent electrons. *Amer. J. Phys., 35,* 26 – 29.

Wybourne, B.G. (1966). Group-theoretical classification of the atomic states of g^N configurations. *J. Chem. Phys., 45,* 1100 – 1104.

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