Terms for Non equivalent Electrons in dxpysz Configurations

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Abstract. jj coupling is predominant in heavier atoms where spin orbit interactions are important than electrostatic interactions. In this manuscript jj coupled terms derived for non equivalent electrons in $d^xp^ys^z$ (x = 1-2, y & z = 0-1) configurations i.e. $d^2 p^1 s^1$, $d^1 p^1 s^1$, $d^1 p^1$ and $d^2 s^1$ configurations, the obtained jj terms are [(5/2, 5/2, 3/2, 1/2), (5/2, 5/2, 1/2, 1/2), (3/2, 3/2, 3/2, 1/2), (3/2, 3/2, 1/2, 1/2), (5/2, 5/2, 3/2, 1/2), (5/2, 5/2, 3/2, 1/2)] for $d^2 p^1 s^1$, [(5/2, 3/2, 1/2), (5/2, 1/2, 1/2), (3/2, 3/2, 1/2), (3/2, 1/2, 1/2)] for $d^1 p^1 s^1$, [(5/2, 3/2), (5/2, 1/2), (3/2, 3/2), (3/2, 1/2)] for $d^1 p^1$ and [(5/2, 5/2, 1/2), (5/2, 3/2, 1/2), (3/2, 3/2, 1/2)] $d^2 s^1$ configurations and the ground state terms determined for these configurations are (3/2, 3/2, 1/2, 1/2), (3/2, 1/2, 1/2), (3/2, 1/2) and (3/2, 3/2, 1/2) respectively.

Key words: Angular momentum, jj coupling, L-S coupling and spin-orbit interaction

INTRODUCTION

LS terms are significant in lower elements which gradually change to jj coupling in going from lighter to heavy atom due to increase nuclear charge (Gauerke and Campbell, 1994). LS terms for equivalent or nonequivalent electrons are derived by different methods i.e. Vector model (Lande, 1921), Quantum mechanical method (Russell & Saunders, 1925) , Ford method (Ford, 1972), Hyde method (Hyde, 1975) , Spin factoring method (McDaniel, 1977), Numerical algorithm method (Kiremire, 1987), Slater graphics (Slater, 1960), Partitioning total spin method (Guofan & Ellzey, 1987), Group representation method (Chen, 1989), Group theoretical method (Wybourne, 1966; Judd, 1967) Generating functions derived via group theory method (Curl & Kilpatrik, 1960), Partial term method (Kiremire, 1990), Partitioning technique(Olson, 2011). The microstate building through electronic arrangement method has been used to generating the spectroscopic LS terms for equivalent electrons of f^3 and f^4 configurations (Meena et al, 2011), and for nonequivalent electrons of $(n-1)f^3nd^1$, $(n-1)f^2nd^1$ and $d^2 p^1 s^1$ configurations (Meena et al 2012 & 2013).

jj terms can also be determine by using different methods which are described by (Rubio and Perez, 1986), (Tuttle, 1967 & 1980), (Haigh, 1990), (Gauerke and Campbell, 1994), (Campbell, 1998), (Novak, 1999), (Orofino and Faria, 2010) and (Richtmyer et al, 1969).

Equivalent electrons have same values of *n* and *l*, the electrostatic interaction is expected to be larger than spin-orbit interaction and L-S coupling is favoured and for nonequivalent, j-j coupling is important. In this manuscript the spectroscopic jj coupled terms for non equivalent electrons of $d^xp^ys^z$ configurations (x= 1-2, y & z= 0-1) were determined and correlated with LS terms (for $d^1 p^1$ and $d^2 s^1$ configuration).

METHODOLOGY

The microstates were built up by arranging electrons with different possible j values for non equivalent electrons of $d^xp^ys^z$ configurations (x= 1-2, y & z = 0-1). Total microstates calculated for $d^2 p^1 s^1$, $d^1 p^1 s^1$, $d^1 p^1$ and $d^2 s^1$ configurations are 540, 120, 60 and 90 respectively**.** Notations for the jj terms designated by the *j*'s are

$[(j_1)^a(j_2)^b(j_3)^c\ldots]$ (Tuttle, 1967 & 1980; Orofino and Faria, 2010) and $[(j_1, j_2)_J]$ (Haigh, 1990). The possible jj terms for non equivalent electrons of $d^xp^ys^z$ configurations (x= 1-2, y & z = 0-1) are [(5/2, 5/2, 3/2, 1/2), (5/2, 5/2, 1/2, 1/2), (3/2, 3/2, 3/2, 1/2), (3/2, 3/2, 1/2, 1/2), (5/2, 3/2, 3/2, 1/2), (5/2, 3/2, 1/2, 1/2), (3/2, 3/2, 1/2, 1/2)] for d^2 p^1 s^1, [(5/2, 3/2, 1/2), (5/2, 1/2, 1/2), $(3/2, 3/2, 1/2)_7$, (3/2, 1/2, 1/2)] for d^1 p^1 s^1, [(5/2, 3/2), [(5/2, 1/2), [(3/2, 3/2), (3/2, 1/2)] for d^1 p^1 and [(5/2, 5/2, 1/2), (5/2, 3/2, 1/2), (3/2, 3/2, 1/2)] for d^2 s^1 configuration.

Microstates for jj Terms for d2 p1 s1 Configuration

The microstate tables for each term is drawn by arranging four electrons and the M_J values for all microstates are determined. The largest M_J value for each term represents a value of J level for term (Table 1). Number of microstates for a particular term of the 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 $\dfrac{(2\ell)!\,(2\ell+2)!}{i!\,(2\ell-i)!\,(n-i)!\,(2\ell+2+i-n)!}$

Table 1: Number of microstates for each jj coupled term for d^2 p^1 s^1 configuration

E1 j_1	E2 j_2	E3 j_3	E4 j_4	jj coupled terms	Microstates	M_J values
5/2	5/2	3/2	1/2	(5/2, 5/2, 3/2, 1/2)	120	6 to -6
5/2	5/2	1/2	1/2	(5/2, 5/2, 1/2, 1/2)	60	5 to -5
3/2	3/2	3/2	1/2	(3/2, 3/2, 3/2, 1/2)	48	4 to -4
3/2	3/2	1/2	1/2	(3/2, 3/2, 1/2, 1/2)	24	3 to -3
5/2	3/2	3/2	1/2	(5/2, 3/2, 3/2, 1/2)	192	6 to -6
5/2	3/2	1/2	1/2	(5/2, 3/2, 1/2, 1/2)	96	5 to -5
Total number of microstates for d^2 p^1 s^1 configuration-540						

J

levels for jj terms for d2 p1 s1 Configuration

J level for jj term are obtained by removing microstates associated with that J level starting from the maximum M_J value in the microstate tables and followed for next levels also.

Table 2: Microstates and their Removal for J Levels for (5/2, 5/2, 3/2, 1/2) Term for d^2 p^1 s^1 configuration

M_J	No. of MS	MS after removing J=6 level	MS after removing J=5(2) levels	MS after removing J=4(3) levels	MS after removing J=3(4) levels	MS after removing J=2 (4) levels	MS after removing J=1(3) levels
6	1	-	-	-	-	-	-
5	3	2	-	-	-	-	-
4	6	5	3	-	-	-	-
3	10	9	7	4	-	-	-
2	14	13	11	8	4	-	-
1	17	16	14	11	7	3	-
0	18	17	15	12	8	4	1
-1	17	16	14	11	7	3	-
-2	14	13	11	8	4	-	-
-3	10	9	7	4	-	-	-
-4	6	5	3	-	-	-	-
-5	3	2	-	-	-	-	-

-6	1	-	-	-	-	-	-
Total	120	107	85	58	30	10	1

For example when the 13 microstates associated with maximum M_J =6 for the jj coupled term (5/2, 5/2, 3/2, 1/2) are eliminated from Table 2 results in J=6 level and maximum M_J level remain is 5 that yield another J=5 level for this term when 22 microstates associated with this are eliminated, and further elimination of 27, 28, 20, 9 and 1 microstates associated with M_J 4, 3, 2, 1 and 0, give 4, 3, 2, 1 and 0 J levels for this term. By applying the same procedure to other terms as illustrated in Table 3 for (5/2, 5/2, 1/2, 1/2) term, Table 4 for (3/2, 3/2, 3/2, 1/2) term, Table 5 for (3/2, 3/2, 1/2, 1/2) term, Table 6 for (5/2, 3/2, 3/2, 1/2) term and Table 7 for (5/2, 3/2, 1/2, 1/2) term.

Table 3: Microstates and their Removal for J Levels for (5/2, 5/2, 1/2, 1/2) Term for d^2 p^1 s^1configuration

M_J	No. of MS	MS after removing J=5 level	MS after removing J=4(2) levels	MS after removing J=3(2) levels	MS after removing J=2(2) levels	MS after removing J=1(2) levels
5	1	-	-	-	-	-
4	3	2	-	-	-	-
3	5	4	2	-	-	-
2	7	6	4	2	-	-
1	9	8	6	4	2	-
0	10	9	7	5	3	1
-1	9	8	6	4	2	-
-2	7	6	4	2	-	-
-3	5	4	2	-	-	-
-4	3	2	-	-	-	-
-5	1	-	-	-	-	-
Total	60	49	31	17	7	1

Table 4: Microstates and their Removal for J Levels for (3/2, 3/2, 3/2, 1/2) Term for d^2 p^1 s^1 configuration

M_J	No. of MS	MS after removing J=4 level	MS after removing J=3(2) levels	MS after removing J=2(3) levels	MS after removing J=1(3) levels
4	1	-	-	-	-
3	3	2	-	-	-
2	6	5	3	-	-
1	9	8	6	3	-
0	10	9	7	4	1
-1	9	8	6	3	-
-2	6	5	3	-	-
-3	3	2	-	-	-
-4	1	-	-	-	-
Total	48	39	25	10	1

Table 5: Microstates and their Removal for J Levels for (3/2, 3/2, 1/2, 1/2) Term for d^2 p^1 s^1 configuration

M_J	No. of M. S.	MS after removing J=3 level	MS after removing J=2(2) levels	MS after removing J=1(2) levels
3	1	-	-	-
2	3	2	-	-
1	5	4	2	-
0	6	5	3	1

-1	5	4	2	-
-2	3	2	-	-
-3	1	-	-	-
Total	24	17	7	1

Table 6: Microstates and their Removal for J Levels for (5/2, 3/2, 3/2, 1/2) Term for d^2 p^1 s^1 configuration

M_J	No. of MS	MS after removing J=6 level	MS after removing J=5(3) levels	MS after removing J=4(5) levels	MS after removing J=3(7) levels	MS after removing J=2(7) levels	MS after removing J=1(5) levels
6	1	-	-	-	-	-	-
5	4	3	-	-	-	-	-
4	9	8	5	-	-	-	-
3	16	15	12	7	-	-	-
2	23	22	19	14	7	-	-
1	28	27	24	19	12	5	-
0	30	29	26	21	14	7	2
-1	28	27	24	19	12	5	-
-2	23	22	19	14	7	-	-
-3	16	15	12	7	-	-	-
-4	9	8	5	-	-	-	-
-5	4	3	-	-	-	-	-
-6	1	-	-	-	-	-	-
Total	192	179	146	101	52	17	2

Table 7: Microstates and their Removal J Levels for (5/2, 3/2, 1/2, 1/2) Term for d^2 p^1 s^1 configuration

M_J	No. of MS	MS after removing J=5 level	MS after removing J=4(3) levels	MS after removing J=3(4) levels	MS after removing J=2(4) levels	MS after removing J=1(3) levels
5	1	-	-	-	-	-
4	4	3	-	-	-	-
3	8	7	4	-	-	-
2	12	11	8	4	-	-
1	15	14	11	7	3	-
0	16	15	12	8	4	1
-1	15	14	11	7	3	-
-2	12	11	8	4	-	-
-3	8	7	4	-	-	-
-4	4	3	-	-	-	-
-5	1	-	-	-	-	-
Total	96	85	58	30	10	1

Number of microstates for jj terms of d^2 s^1 configuration

1. Term (5/2, 5/2, 1/2) or [$(d_{5/2})^2 (s_{1/2})^1$]

$$\frac{(2\,x\,2)!\,(2\,x\,2\;+\;2)!}{0!\,(2x\;2\;-\;0)!\;(2\;-\;0)!\;(2\,x\,2\;+\;2\;+\;0\;-\;2)!}\;x\;\frac{(0x2)!\,(0x2+2)!}{0!\,(0x\,2-0)!\,(1-0)!\,(0x2+2+0-1)!}=30$$

2. Term (5/2, 3/2, 1/2) or [$(d_{5/2})^1 (d_{3/2})^1 (s_{1/2})^1$]

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

3. Term (3/2, 3/2, 1/2) or [$(d_{3/2})^2 (s_{1/2})^1$]

$$\frac{(2\,x\,2)!\,(2\,x\,2\;+\;2)!}{2!\,(2x\;2\;-\;2)!\;(2\;-\;2)!\;(2\,x\,2\;+\;2\;+\;2\;-\;2)!}\;x\;\frac{(0x2)!\,(0x2+2)!}{0!\,(0x\,2-0)!\,(1-0)!\,(0x2+2+0-1)!}=12$$

Number of microstates for jj terms of d1 p1 s1 configuration

1. Term (5/2, 3/2, 1/2) or [$(d_{5/2})^1 (p_{3/2})^1 (s_{1/2})^1$]

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

2. Term (3/2, 3/2, 1/2) or [$(d_{3/2})^1 (p_{3/2})^1 (s_{1/2})^1$]

$$\frac{(2x2)!(2x2+2)!}{1!\,(2x\,2-1)!\,(1-1)!\,(2x2+2+1-1)!}\;x\;\frac{(1x2)!(1x2+2)!}{0!\,(1x\,2-0)!\,(1-0)!\,(1x2+2+0-1)!}\;x\;\frac{(0x2)!(0x2+2)!}{0!\,(0x\,2-0)!\,(1-0)!\,(0x2+2+0-1)!}=32$$

3. Term (5/2, 1/2, 1/2) or [$(d_{5/2})^1 (p_{1/2})^1 (s_{1/2})^1$]

$$\frac{(2x2)!(2x2+2)!}{0!\,(2x\,2-0)!\,(1-0)!\,(2x2+2+0-1)!}\;x\;\frac{(1x2)!(1x2+2)!}{1!\,(1x\,2-1)!\,(1-1)!\,(1x2+2+1-1)!}\;x\;\frac{(0x2)!(0x2+2)!}{0!\,(0x\,2-0)!\,(1-0)!\,(0x2+2+0-1)!}=24$$

4. Term (3/2, 1/2, 1/2) or [$(d_{3/2})^1 (p_{1/2})^1 (s_{1/2})^1$]

$$\frac{(2x2)!(2x2+2)!}{1!\,(2x\,2-1)!\,(1-1)!\,(2x2+2+1-1)!}\;x\;\frac{(1x2)!(1x2+2)!}{1!\,(1x\,2-1)!\,(1-1)!\,(1x2+2+1-1)!}\;x\;\frac{(0x2)!(0x2+2)!}{0!\,(0x\,2-0)!\,(1-0)!\,(0x2+2+0-1)!}=16$$

Number of microstates for jj terms of d1 p1 configuration

1. Term (5/2, 3/2) or [$(d_{5/2})^1 (p_{3/2})^1$]

$$\frac{(2x2)!(2x2+2)!}{0!\,(2x\,2-0)!\,(1-0)!\,(2x2+2+0-1)!}\;x\;\frac{(1x2)!(1x2+2)!}{0!\,(1x\,2-0)!\,(1-0)!\,(1x2+2+0-1)!}=24$$

2. Term (3/2, 3/2) or [$(d_{3/2})^1 (p_{3/2})^1$]

$$\frac{(2x2)!(2x2+2)!}{1!\,(2x\,2-1)!\,(1-1)!\,(2x2+2+1-1)!}\;x\;\frac{(1x2)!(1x2+2)!}{0!\,(1x\,2-0)!\,(1-0)!\,(1x2+2+0-1)!}=18$$

3. Term (5/2, 1/2) or [$(d_{5/2})^1 (p_{1/2})^1$]

$$\frac{(2x2)!(2x2+2)!}{0!\,(2x\,2-0)!\,(1-0)!\,(2x2+2+0-1)!}\;x\;\frac{(1x2)!(1x2+2)!}{1!\,(1x\,2-1)!\,(1-1)!\,(1x2+2+1-1)!}=12$$

4. Term (3/2, 1/2) or $[(d_{3/2})^1 (p_{1/2})^1]$

$$\frac{(2x2)!(2x2+2)!}{1!(2x2-1)!(1-1)!(2x2+2+1-1)!}\ x\ \frac{(1x2)!(1x2+2)!}{1!(1x2-1)!(1-1)!(1x2+2+1-1)!} = 8$$

By applying same method as used for d^2 p^1 s^1 configuration J levels are determined which are $[(5/2, 3/2, 1/2)_{9/2, 7/2(2), 5/2(2), 3/2(2), 1/2}]$, $[(5/2, 1/2, 1/2)_{7/2, 5/2(2), 3/2}]$, $[(3/2, 3/2, 1/2)_{7/2, 5/2(2), 3/2(2), 1/2(2)}]$ and $[(3/2, 1/2, 1/2)_{5/2, 3/2(2), 1/2}]$ for d^1 p^1 s^1 configuration, $[(5/2, 3/2)_{4, 3, 2, 1}]$, $[(5/2, 1/2)_{3, 2}]$, $[(3/2, 3/2)_{3, 2, 1, 0}]$ and $[(3/2, 1/2)_{2, 1}]$ for d^1 p^1 configuration and $[(5/2, 5/2, 1/2)_{9/2, 7/2, 5/2, 3/2, 1/2}]$, $[(5/2, 3/2, 1/2)_{9/2, 7/2(2), 5/2(2), 3/2(2), 1/2}]$ and $[(3/2, 3/2, 1/2)_{5/2, 3/2, 1/2}]$ for d^2 s^1 configuration.

RESULTS AND DISCUSSION

jj coupled spectroscopic terms obtained for $d^xp^ys^z$ configurations (x= 1-2, y & z = 0-1) are $[\{(5/2, 5/2, 3/2, 1/2)_{6, 5(2), 4(3), 3(4), 2(4), 1(3), 0}\}$, $\{(5/2, 5/2, 1/2, 1/2)_{5, 4(2), 3(2), 2(2), 1(2), 0}\}$, $\{(3/2, 3/2, 3/2, 1/2)_{4, 3(2), 2(3), 1(3), 0}\}$, $\{(3/2, 3/2, 1/2, 1/2)_{3, 2(2), 1(2), 0}\}$, $\{(5/2, 3/2, 3/2, 1/2)_{6, 5(3), 4(5), 3(7), 2(7), 1(5), 0(2)}\}$,$\{(5/2, 3/2, 1/2, 1/2)_{5, 4(3), 3(4), 2(4), 1(3), 0}\}]$ for d^1 p^1 s^1 configuration, $[\{(5/2, 3/2, 1/2)_{9/2, 7/2(2), 5/2(2), 3/2(2), 1/2}\}$, $\{(5/2, 1/2, 1/2)_{7/2, 5/2(2), 3/2}\}$, $\{(3/2, 3/2, 1/2)_{7/2, 5/2(2), 3/2(2), 1/2(2)}\}$, $\{(3/2, 1/2, 1/2)_{5/2, 3/2(2), 1/2}]$ for d^2 p^1 s^1 configuration, $[\{(5/2, 3/2)_{4, 3, 2, 1}\}$, $\{(5/2, 1/2)_{3, 2}\}$, $\{(3/2, 3/2)_{3, 2, 1, 0}\}$, $\{(3/2, 1/2)_{2, 1}\}]$ for d^1 p^1 configuration and $[\{(5/2, 5/2, 1/2)_{9/2, 7/2, 5/2, 3/2, 1/2}\}$, $\{(5/2, 3/2, 1/2)_{9/2, 7/2(2), 5/2(2), 3/2(2), 1/2}\}$, $\{(3/2, 3/2, 1/2)_{5/2, 3/2, 1/2}\}]$ for d^2 s^1 configuration.

And the ground state jj coupled terms determined for these configurations are $[(3/2, 3/2, 1/2, 1/2)_{3, 2(2), 1(2), 0}]$, $[(3/2, 1/2, 1/2)_{5/2, 3/2(2), 1/2}]$, $[(3/2, 1/2)_{2, 1}]$ and $[(3/2, 3/2, 1/2)_{5/2, 3/2, 1/2}]$ respectively. In correlation level diagram the L-S and the j-j levels for d^1 p^1 and d^2 s^1 configurations are shown (Figure 1 and Figure 2). Total number of final states are same, but their relative energies are different.

CONCLUSION

Here a simple and systematic method is described to obtain the jj coupled spectroscopic terms for nonequivalent electrons of $d^xp^ys^z$ configurations (x= 1-2, y & z= 0-1). For d^2 p^1 s^1, d^1 p^1 s^1, d^1 p^1 and d^2 s^1 configurations, this procedure will make jj coupled terms more popular in chemistry and also helpful to investigate the atomic and electronic spectra of nonequivalent electron containing atoms or free ions.

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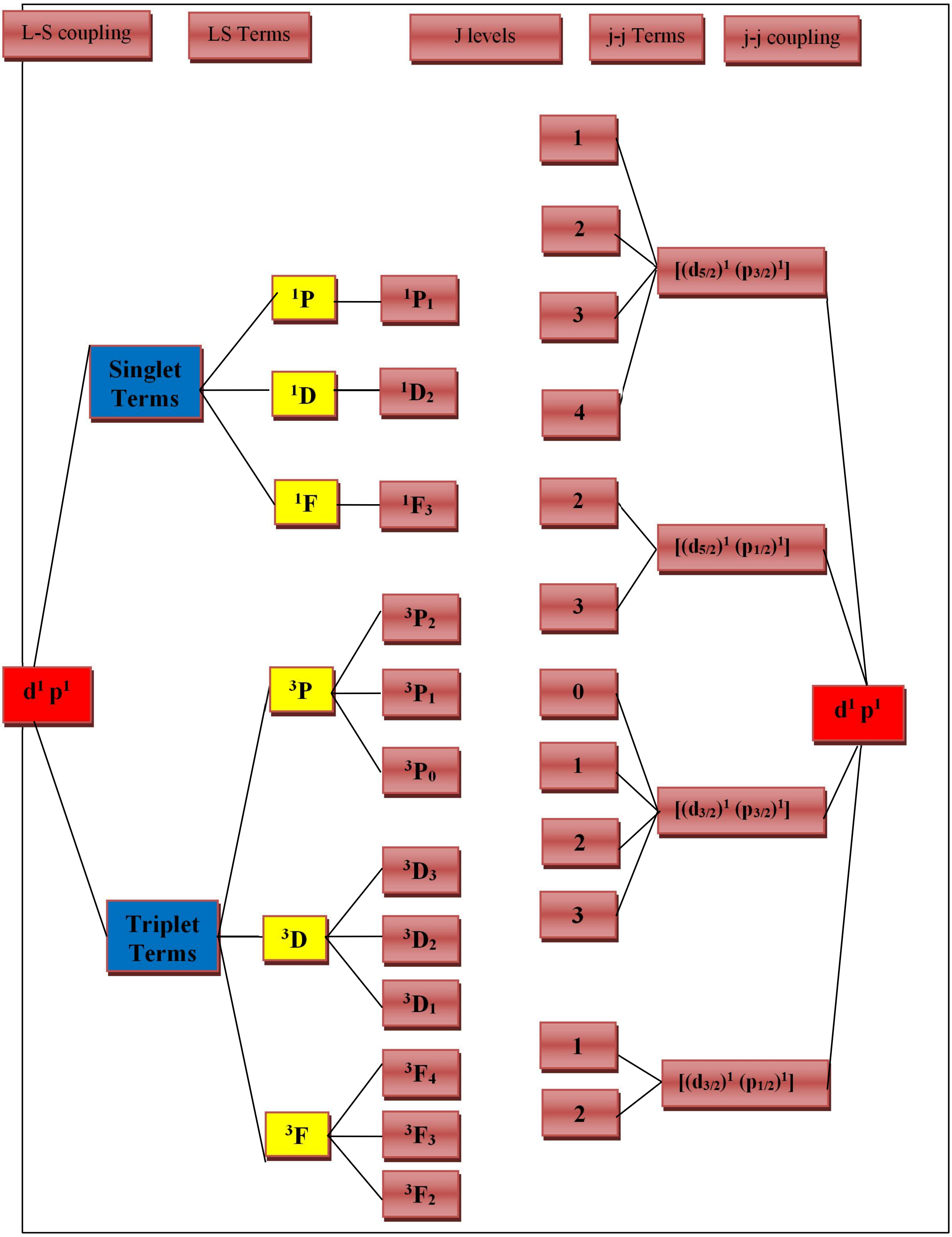

Figure1: Correlation diagram for LS and jj coupling schemes for levels for d^1 p^1 configuration

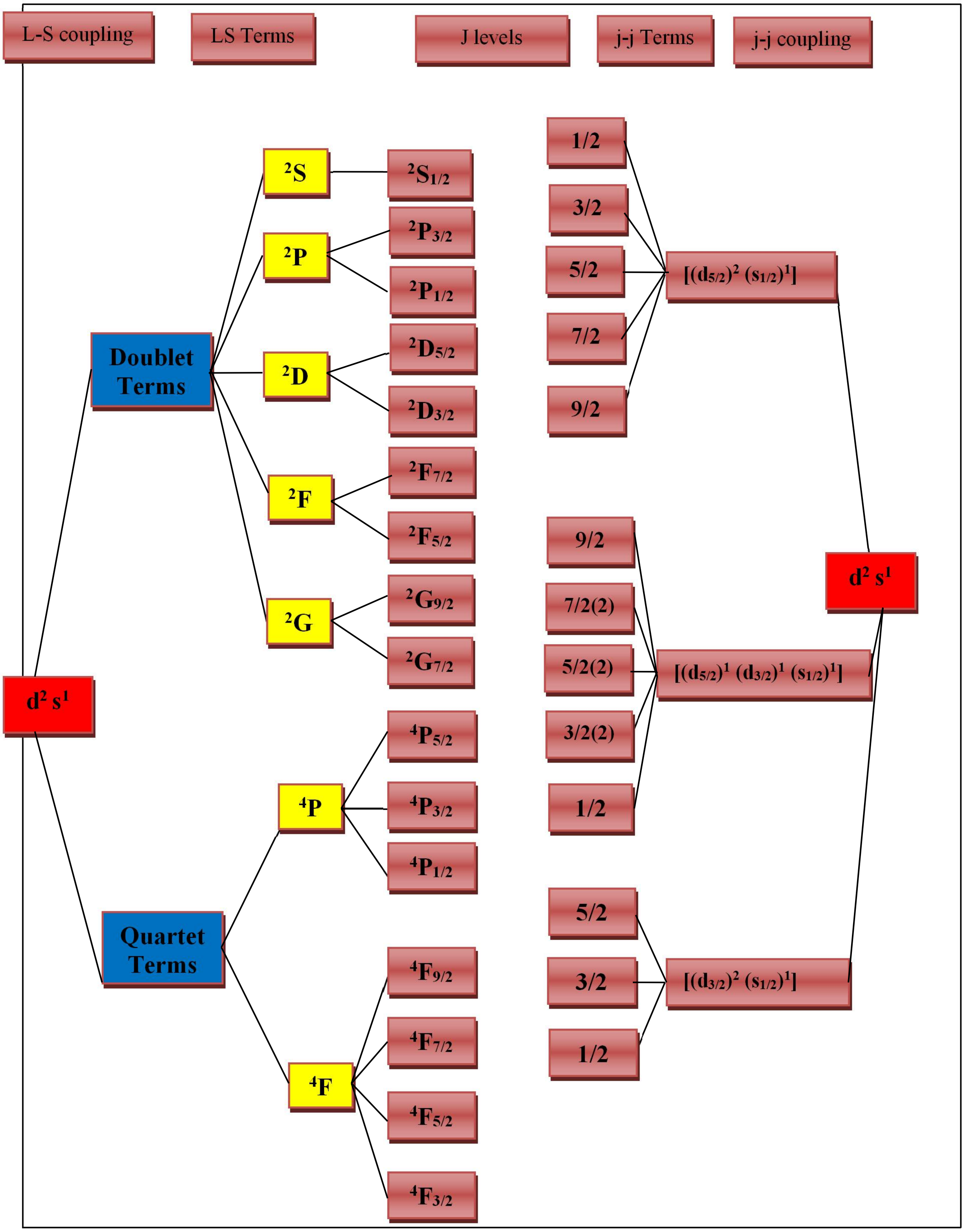

Figure 2: Correlation diagram for LS and jj coupling schemes for levels for $d^2 s^1$ configuration