jj Terms for Non equivalent Electrons in $d^xp^ys^z$ 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.

Keywords*:* 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 & 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., 2011a; 2011b), 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; Meena et al., 2013).

jj terms can also be determine by using different methods which are described by (Rubio & Perez, 1986), (Tuttle, 1967), (Haigh, 1990), (Gauerke & Campbell, 1994), (Campbell, 1998), (Novak, 1999), (Orofino & Faria, 2010), (Richtmyer et al, 1969) and (Meena et al., 2015). 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 an d correlated with LS terms (for $d^1 p^1$ and $d^2 s^1$ configuration).

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Methodology

The microstates were built up by arranging electrons with different possible j values for non equivalent electrons of $d^x p^y s^z$ 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 & Faria, 2010) and $[(j_1, j_2)_J]$ (Haigh, 1990). The possible jj terms for non equivalent electrons of $d^x p^y s^z$ 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 d^2 p^1 s^1 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 A1). 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

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

J levels for jj terms for d^2 p^1 s^1 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. 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 A2 results in J=6 level and maximum M_J level remain is 5 that yield another J=5 level for this term when 22 microstat 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 A3 for (5/2, 5/2, 1/2, 1/2) term, Table A4 for (3/2, 3/2, 3/2, 1/2) term, Table A5 for (3/2, 3/2, 1/2, 1/2) term, Table A6 for (5/2, 3/2, 3/2, 1/2) term and Table A7 for (5/2, 3/2, 1/2, 1/2) term.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Number of microstates for jj terms of d^1 p^1 configuration

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

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

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

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

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

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

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 numbers of final states are same, but their relative energies are different.

CONCLUSSION

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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Appendix A

Table A1

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						

Table A2

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

Table A3

Microstates and their Removal for J Levels for (5/2, 5/2, 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(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 A4

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 A5

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 A6

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 A7

Microstates and their Removal for 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

Appendix B

Figure B1

Correlation Diagram for LS and jj Coupling Schemes for Levels for $d^1\,p^1$ Configuration

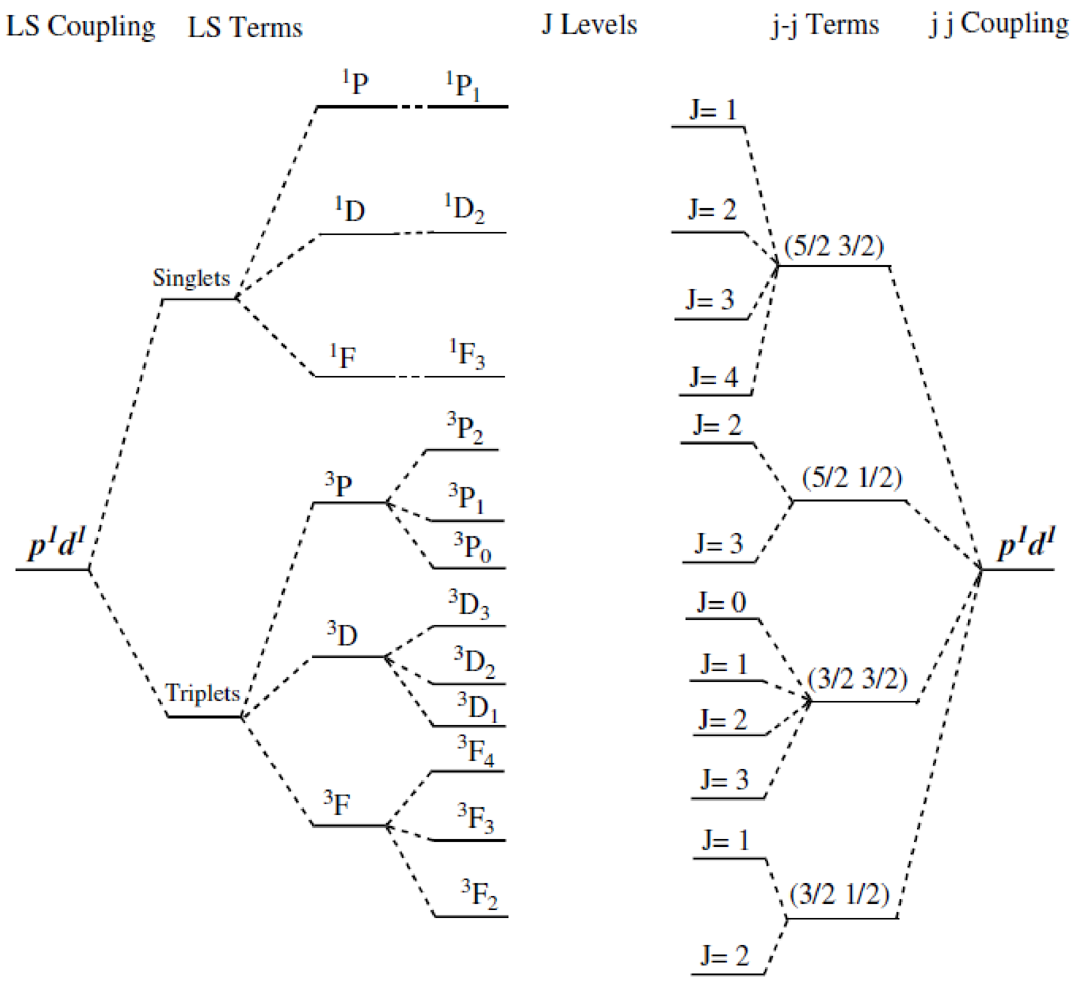

Figure B2

Correlation Diagram for LS and jj Coupling Schemes for Levels for $d^2 s^1$ Configuration