Determination of spectral term for L-S coupling:→

example (a) Atoms with one optical electron i.e 1s

Here $l = 0, s = \frac{1}{2}$, $S = 2s+1 = 2\times\frac{1}{2}+1 = 2$

$J = (l \pm s) = \frac{1}{2}$

⇒ Term value $= {}^{2s+1}A_J = {}^{2}S_{1/2}$ as $l = 0$ ⇒ S state, $J = \frac{1}{2}$

(b) Atom with two non equivalent optical electron

Non-equivalent e^- have different 'n' & l value.

$2p\,3d \rightarrow l_1 = 1,\ l_2 = 2,\ s_1 = \frac{1}{2},\ s_2 = \frac{1}{2}$

$s = (s_1 \pm s_2) = 0, 1$ $S = 2s+1 = 2\times0+1 = 1$ (singlet)
$= 2\times1+1 = 3$ (triplet)

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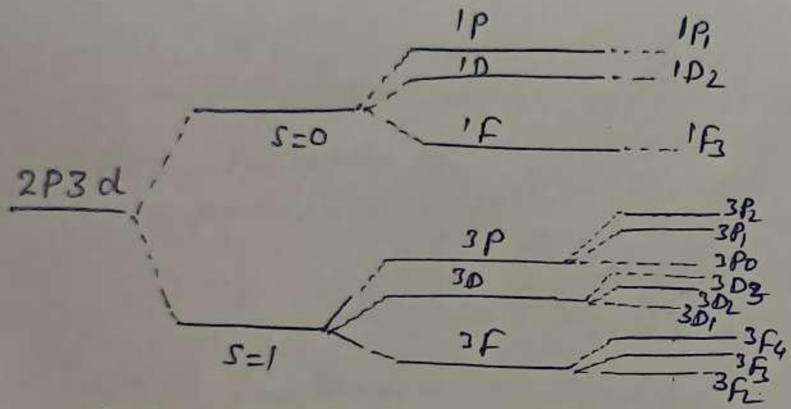
$l_1 = 1,\ l_2 = 2 \quad L = |l_1 \pm l_2| = 1, 2, 3 \quad (P, D, F)$

$J = |L \pm S| = 1+0 = 1$
$2+0 = 2 \quad S = 0,\ 2S+1 = 1$
$3+0 = 3$

$J = 2 \pm 1 = 1, 2, 3$
$3 \pm 1 = 1, 2, 3, 4 \quad S = 1$
$1 \pm 1 = 0, 1, 2$

Non equivalent optical electrons :–
The electrons having different 'n' & 'l' values are known as non equivalent optical electrons e.g.
2P, 3d $\quad n = 2, 3,\ l = 1, 2$

Equivalent optical electrons
The electrons having same value of 'n' & 'l' is known as equivalent electrons
e.g. $2P^2 \quad n = 2,\ l = 1$ for both of the optical e–



Degeneracy of level 2P3d

Degeneracy is calculated with the formula $(2J+1)$

for $^1P_1$, $J=1$, degeneracy $= 2J+1 = 2\times1+1 = 03$
$^1D_2$, $J=2$ 〃 $= 2J+1 = 2\times2+1 = 05$
$^1F_3$, $J=3$ 〃 $= 2J+1 = 2\times3+1 = 07$
$^3P_2$, $J=2$ 〃 $= 2\times J+1 = 2\times2+1 = 05$
$^3P_1$, $J=1$ 〃 $= 2J+1 = 2\times1+1 = 03$
$^3P_0$, $J=0$ 〃 $= 2J+1 = 2\times0+1 = 01$
$^3D_3$, $J=3$ 〃 $= 2\times3+1 = 2\times3+1 = 07$
$^3D_2$, $J=2$ $= 2J+1 = 2\times2+1 = 05$
$^3D_1$, $J=1$ $= 2J+1 = 2\times1+1 = 03$
$^3F_4$, $J=4$ 〃 $= 2J+1 = 2\times4+1 = 09$
$^3F_3$, $J=3$ $= 2J+1 = 2\times3+1 = 07$
$^3F_2$, $J=2$ $= 2J+1 = 2\times2+1 = 05$

Total degeneracy = 60
The degeneracy can be removed when an atom is placed in external magnetic field.

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MPHYCC10-09

* closed subshell like s^2, p^6, d^{10}, f^{14} will give rise to $^1S_0$ term
* closed subshell contains maximum number of electrons $= 2(2l+1)$

example s^2 $l = 0$, no of electrons $= 2(2\times0+1) = 2$
p^6 $l = 1$,, $= 2(2\times1+1) = 2(3) = 6$

* The term can be odd/even when $\Sigma l =$ odd/even
example $4p4d$, $l_1 = 1, l_2 = 2$ $\Sigma l = 1+2 = 03$ odd then we can write the term as $^1P^o, {}^1D^o, {}^1F^o, {}^3P^o, {}^3D^o, {}^3F^o$

Term value determination of equivalent e^-s. :-

Rule :- The terms of configuration $(nl)^q$ are same as the terms of the configuration $(nl)^{r-q}$ $r =$ maximum number of e^-s
$r = 2(2l+1)$

Term of p^1 is similar to p^5
p^q is similar to p^{r-q}

for p subshell $l = 1$
maximum no of $e^- = 2(2l+1)$
$r = 2(2\times1+1)$
$r = 6$

$q=1$ given p^1 ∴ $p^{6-1} = p^5$

Term of p^1 is similar to p^5

Question (i) p^2 is similar to ---- ?
(ii) d^2 is similar to ----- ?
(iii) d^8 is similar to ---- ?
(iv) p^4 is similar to ---- ?

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Determination of term values for equivalent electrons :→

$(nd)^2$ n & l are same for both of the electrons hence these are termed as equivalent electrons.

$s_1 = \frac{1}{2}$, $s_2 = \frac{1}{2}$ $S = s_1 \pm s_2 = 0, 1$.

$l_1 = 2$, $l_2 = 2$ $L = |l_1 \pm l_2| = 0, 1, 2, 3, 4$
S P D F G

Now According to Breit's scheme the possible values of M_L is

m_{l_1}	2	1	0	-1	-2	
M_L	4	3	2	-1	0	2
M_L	3	2	1	0	-1	1
M_L	2	1	0	-1	-2	0
M_L	1	0	-1	-2	-3	-1
M_L	0	-1	-2	-3	-4	-2

4, 3, 2, 1 0 -1, -2, -3, -4 — G L=4
3, 2, 1, 0 -1, -2, -3 — F L=3
2, 1, 0, -1, -2 — D L=2
1, 0, -1 ⟶ P L=1
0 ⟶ S L=0

for S=1, L = 3 & L = 1
S = 0, L = 4, 2, 0

Possible states are ^1G, ^3F, ^1D, ^3P, ^1S

^1G = L = 4, S = 0 ⇒ $^1G_4$
^1D = L = 2, S = 2 ⇒ $^1D_2$
^1S = L=0, S=0 ⇒ $^1S_0$

^3P, L = 1, S = 1 J = |1±1| = 0, 1, 2
$^3P_{0,1,2}$
^3F, L = 3, S = 1, J = |1±3| = 2, 3, 4
$^3F_{2,3,4}$

The term value for $(nP)^2$ state will be $^1G_4$, $^3F_{2,3,4}$, $^1D_2$, $^3P_{0,1,2}$, $^1S_0$

the terms of $(nP)^2$ will be similar to $(nP)^4$

Therefore the terms of $(nP)^4$ will be $^1G_4$, $^3F_{2,3,4}$, $^1D_2$, $^3P_{0,1,2}$, $^1S_0$

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MPHYCC10 — 09

Determination of term value of $(nd)^2$ configuration: similar to $l = 2$ for $(np)^2$: the electrons are equivalent as n is similar & $l = 1$ for both the e^-s.

$s_1 = \frac{1}{2}$, $s_2 = \frac{1}{2}$ $\Rightarrow S = |s_1 \pm s_2| = 0, 1$

$l_1 = 1$, $l_2 = 1$ $\Rightarrow L = |l_1 \pm l_2| = 0, 1, 2$ ~~3, 4~~
S, P, D ~~F, G~~

Possible M_L values from Breit's scheme:—

m_{l_2} \ m_{l_1}	1	0	−1
1	2	1	0
0	1	0	−1
−1	0	−1	−2

2 1 0 −1 −2
1 0 −1
0

for $S = 1$, $M_L = 1, 0, -1$, $L = 1$
$J = |L \pm S| = 0, 1, 2$
$^3P_{0,1,2}$

for $S = 0$, $M_L = 2, 1, 0, -1, -2$, $L = 2$
$M_L = 0$ $L = 0$

$S = 0, L = 0, J = 0$
$S = 0, L = 2, J = 2$

$^1S_0$, $^3P_{0,1,2}$, $^1D_2$

The term value for $(np)^2$ electron is $^1S_0$, $^3P_{0,1,2}$, $^1D_2$

Question :- Determine the term values for $(np)^4$