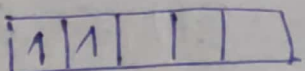
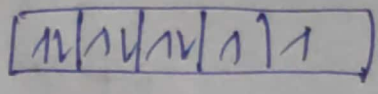
Correlation and spin-orbit coupling in Free ions for First series of Transition Metal :—

2. V^{3+} and Ni^{2+} (d^2, d^8) :—

V^{3+} – d^2 

Ni^{2+} – d^8 

Both have 2 unpaired electron.

V^{3+} d^2 No. of microstate $= (n/r) = \frac{n!}{r!(n-r)!}$

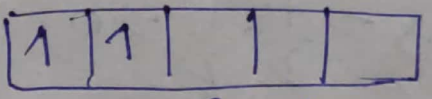
$= \left(\frac{10}{2}\right) = \frac{10!}{2!(10-2)!}$

$= \frac{10\times9\times8\times7\times6\times5\times4\times3\times2\times1}{2\times1(8\times7\times6\times5\times4\times3\times2\times1)}$

$= \frac{90}{2} = 45$ microstate.

Both have 45 microstate.

Term symbol for d^2



$S = \frac{1}{2} + \frac{1}{2} = 1$

$L = 2+1 = 3$

Term symbol = F

spin multiplicity $= 2S+1$

$= 2\times1+1 = 3$

Term symbol – $^{2S+1}L_J$

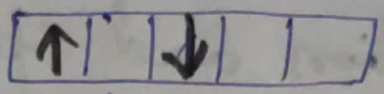
$J = L+S = 3+1 = 4$

$L+S-1 = 4-1 = 3$

$L+S-2 = 4-2 = 2$

$^3F_4$ $^3F_3$ $^3F_2$

$^3F_4$ ground state



$S = \frac{1}{2} + \frac{1}{2} = 0$

$L = 2+0 = 2$

Term - D

Spin multiplicity $2S+1 = 2\times0+1 = 1$

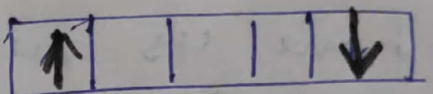
Term symbol = ^1D

$S = \frac{1}{2} + \frac{1}{2} = 1$

$L = 1+0 = 1$

Spin multiplicity $= 2S+1 = 2\times1+1 = 3$

Term symbol. ^3P



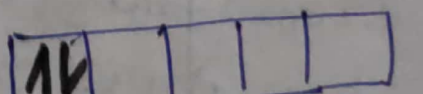
$S = \frac{1}{2} - \frac{1}{2} = 0$

$L = 2-2 = 0$

Term = S

Spin multiplicity $= 2S+1 = 2\times0+1 = 1$

Term symbol ^1S



$S = \frac{1}{2} - \frac{1}{2} = 0$

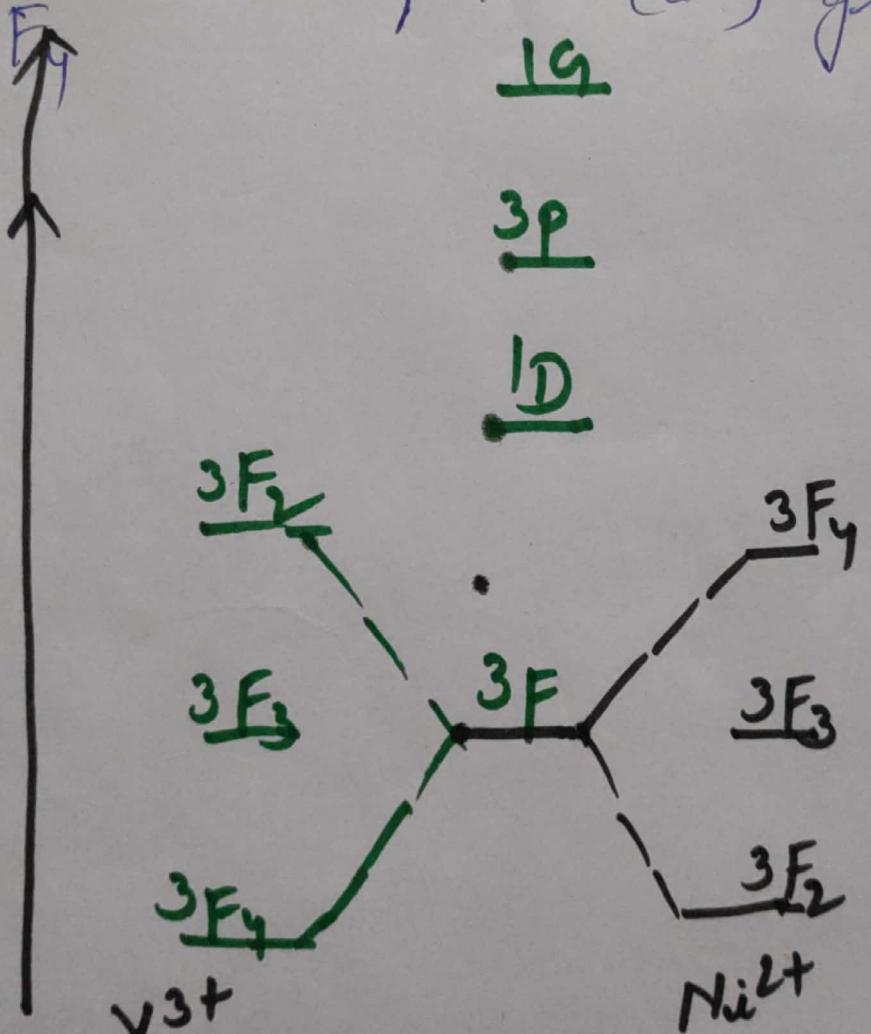
$L = 2+2 = 4$

Term - G

Spin multiplicity $2S+1 = 2\times0+1 = 1$

Term symbol = ^1G

Therefore in d^2 system due to 45 microstates we get following term symbol. ^3F, ^1D, ^3P, ^1S, ^1G and ^3F is the ground term. Due to L-S coupling ^3F term split in to $^3F_2$, $^3F_3$, $^3F_4$ in case of $V^{3+}(d^2)$ ground term is $^3F_2$ in case of $Ni^{2+}(d^8)$ ground term is $^3F_4$



Correlation and spin orbit coupling of free ion V^{3+} and Ni^{2+}