# Microstate/Term & Symbol

## M. Sc. Inorganic Chemistry
## CC-1/CC-6/NET/PAT

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# Microstate

Microstate is the arrangement of electron of particular electronic configuration which can be differentiated in terms of energy or angular momentum.

it is energy (states) level of different arrangement of electron.

We know that there is motionable energy (rotational, vibrational & translational energy) & it gives S-S interaction (coupling) l-l coupling & j-j coupling which gives several types of energy states (level).

It is calculated by following formula

$$\text{No. of Microstate} = \frac{n!}{e!\,(n-e)!}$$

n = twice of the no. of orientation of orbital

e = No. of given e-

But some of it are allowable & some are not

Let us consider $P^1$ system which have 6 possible arrangement like this

| | $p_x$ | $p_y$ | $p_z$ |
|---|---|---|---|
| 1 | ↑ | | |
| 2 | ↓ | | |
| 3 | | ↑ | |
| 4 | | ↓ | |
| 5 | | | ↑ |
| 6 | | | ↓ |

Similarly for $d^x$ system microstates are as

**Microstates for $nd^{1-10}$**

| configuration | $d^1$ | $d^2$ | $d^3$ | $d^4$ | $d^5$ | $d^6$ | $d^7$ | $d^8$ | $d^9$ | $d^{10}$ |
|---|---|---|---|---|---|---|---|---|---|---|
| microstates | 10 | 45 | 120 | 210 | 252 | 210 | 120 | 45 | 10 | 1 |

The number of microstates (the total degeneracy) for a configuration $nd^x$ is the same as for $nd^{10-x}$.

# Term Symbol & State

Term Symbol & state are the abbreviated form of electronic configuration bearing low energy orbital of the system. Term symbol of an electron arrangement reflects the total spin angular momentum(Ms), total orbital angular momentum(L) & total angular momentum(J). It is represented by following formula

Ms

L

J

Where

Ms= 2S+1 (S=total spin quantum no.)=total spin angular momentum. It gives idea of s-s coupling.

S=s1+s2+……….. For $P^2$ system s=+1/2+1/2=1

So Ms = 2x1+1=3

| Microstate index | $m_l$ +1 | 0 | -1 | $M_S$ |
|---|---|---|---|---|
| 1 | ↑ | ↑ | | +1 |
| 2 | | ↑ | ↑ | +1 |
| 3 | ↑ | | ↑ | +1 |
| 4 | ↓ | ↓ | | -1 |
| 5 | | ↓ | ↓ | -1 |
| 6 | ↓ | | ↓ | -1 |
| 7 | ↑ | ↓ | | 0 |
| 8 | ↑ | | ↓ | 0 |
| 9 | ↓ | ↑ | | 0 |
| 10 | | ↑ | ↓ | 0 |
| 11 | ↓ | | ↑ | 0 |
| 12 | | ↓ | ↑ | 0 |
| 13 | ↑↓ | | | 0 |
| 14 | | ↑↓ | | 0 |
| 15 | | | ↑↓ | 0 |

At 1$^{st}$ maximum Ms gives maximum stability & then maximum L value gives maximum stability

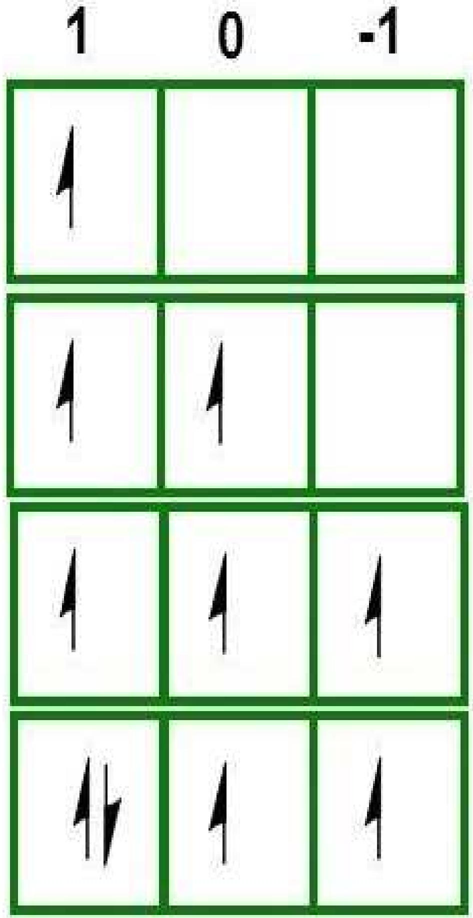
L= total orbital angular momentum=term

It gives idea about l-l coupling. It represents term

| L = | 0 | 1 | 2 | 3 |
|---|---|---|---|---|
| Term = | S | P | D | F |

| Microstate index | $m_l$ +1 | 0 | -1 | $L$ |
|---|---|---|---|---|
| 1 | ↑ | ↑ | | +1 |
| 2 | | ↑ | ↑ | -1 |
| 3 | ↑ | | ↑ | 0 |
| 4 | ↓ | ↓ | | +1 |
| 5 | | ↓ | ↓ | -1 |
| 6 | ↓ | | ↓ | 0 |
| 7 | ↑ | ↓ | | +1 |
| 8 | ↑ | | ↓ | 0 |
| 9 | ↓ | ↑ | | +1 |
| 10 | | ↑ | ↓ | -1 |
| 11 | ↓ | | ↑ | 0 |
| 12 | | ↓ | ↑ | -1 |
| 13 | ↑↓ | | | +2 |
| 14 | | ↑↓ | | 0 |
| 15 | | | ↑↓ | -2 |

- Draw out $2l+1$ boxes and label with $m_l$ values
  - Place electrons in boxes to maximize S (1st Rule)
  - Occupy from left to right to maximize L (2nd Rule)
  - Add $m_s$ to get S and $m_l$ to get L




$p^1$: $L = 1, S = \frac{1}{2} \rightarrow 2S+1 = 2 \rightarrow {}^2P$

$p^2$: $L = 1, S = \frac{1}{2} + \frac{1}{2} = 1 \rightarrow 2S+1 = 3 \rightarrow {}^3P$

$p^3$: $L = 0, S = 3 \times \frac{1}{2} = 3/2 \rightarrow 2S+1 = 4 \rightarrow {}^4S$

$p^4$: $L = 1, S = \frac{1}{2} + \frac{1}{2} = 1 \rightarrow 2S+1 = 3 \rightarrow {}^3P$

Energy level of different terms of given electronic configuration can be arranged by certain rules. Let us consider following example

$d^2$ electron configuration

Two electrons in $d_{xy}$, $d_{xz}$, $d_{xy}$, $d_{z2}$ and $d_{x2-y2}$ orbitals.

$^1G$ $^3F$ $^1D$ $^3P$ $^1S$

1. For a given electron configuration, the term with the greatest multiplicity lies lowest in energy. (Hund's rule.)
2. For a term of a given multiplicity, the greater the value of L, the lower the energy.

Lowest E — Highest E

$^3F < {}^3P < {}^1G < {}^1D < {}^1S$

Note: The rules for predicting the ground state always work, but they may fail in predicting the order of energies for excited states.

Lowest E — Highest E

Real Order $^3F < {}^1D < {}^3P < {}^1G < {}^1S$

J=L+S to L-S it gives idea about LS coupling for less than half filled less value of J(=L-S) value is effective & more than half filled more value of J(=L+S) is effective

# How to find Microstates

## Type -1

### When electronic configuration in 1 suborbit is given

$$\text{No. of Micro State} = \frac{|\underline{n}}{|\underline{e}\;\; |\underline{n-e}}$$

n = twice the no. of orbital

e = No. of given e-

Example

$$P^1 = \frac{|\underline{6}}{|\underline{1}\;\; |\underline{6-1}} = 6$$

$$P^2 = \frac{|\underline{6}}{|\underline{2}\;\; |\underline{6-4}} = 15$$

**Microstates for $nd^{1-10}$**

| configuration | $d^1$ | $d^2$ | $d^3$ | $d^4$ | $d^5$ | $d^6$ | $d^7$ | $d^8$ | $d^9$ | $d^{10}$ |
|---|---|---|---|---|---|---|---|---|---|---|
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The number of microstates (the total degeneracy) for a configuration $nd^x$ is the same as for $nd^{10-x}$.

# Type - II

## Electronic configuration in two suborbits are given

$$\text{No. of Microstate} = \frac{n!}{e!\,(n-e)!} \times \frac{n!}{e!\,(n-e)!}$$

For $P^1$ For $d^1$

Example

$$6 \text{ X } \frac{10!}{1!\,(10-1)!} = 6\text{X}10 = 60$$

# Type - III

## When term symbol are given

$(2S+1)_L$

Formula = 2S+1 X 2L+1

for $2_D$ , 2S+1= 2 & 2L+1=2x2+1=5

No. Of M.S. = 2X5=10

For 3F

2S+1=3 & 2L+1=2x3+1=7

No. of microstate=3x7=21

# Type - IV

## When ground term state(GST) is given

$^{(2S+1)}L_J$

**Formula = (2J+1)**

J = L + S: number of microstates = 2J + 1

$^3P_2$ (5 microstates)
$^3P_1$ (3 microstates) 9 microstates
$^3P_0$ (1 microstate)

| | | | |
|---|---|---|---|
| For | $^1G \rightarrow {}^1G_4$ | (L = 4, S = 0) | 9 microstates |
| | $^1S \rightarrow {}^1S_0$ | (L = 0, S = 0) | 1 microstate |
| | $^1D \rightarrow {}^1D_2$ | (L = 2, S = 0) | 5 microstates |
| | $^3F \rightarrow {}^3F_4$ | (L = 3, S = 1) | 9 microstates |
| | $^3P \rightarrow {}^3P_2$ | (L = 1, S = 1) | 5 microstates |

# Type - V

## When degeneracy is given

No. of microstate = 2S+1 X degeneracy

Here

| Degeneracy | Singlet | Doublet | Triplet |
|---|---|---|---|
| | A(1) | E(2) | T(3) |

$^{2}T_{1g}$

Here 2S+1=2 & degeneracy for T=3

So no. of microstate= 2S+1 x degeneracy=2x3=6

$3T_{2g}$

Formula = $(2S+1)_L$

= 3X3=9

$2A_{1g}$

No. of microstate= 2X1=2

# Thank You