Atomic states derived from electronic configuration

There are two ways to set J

1- The first method (LS coupling)

is used when the spin motion does not couple much with the angular momentum of the orbital L of each electron with the rest, resulting in a single resultant symbolized by the quantum letter for that case. Also, the spin momentum of each electron couples with the rest, resulting in a resultant momentum S and L values, S of all the spin motions, which are symbolized by the quantum letter

2-The second method (jj coupling)

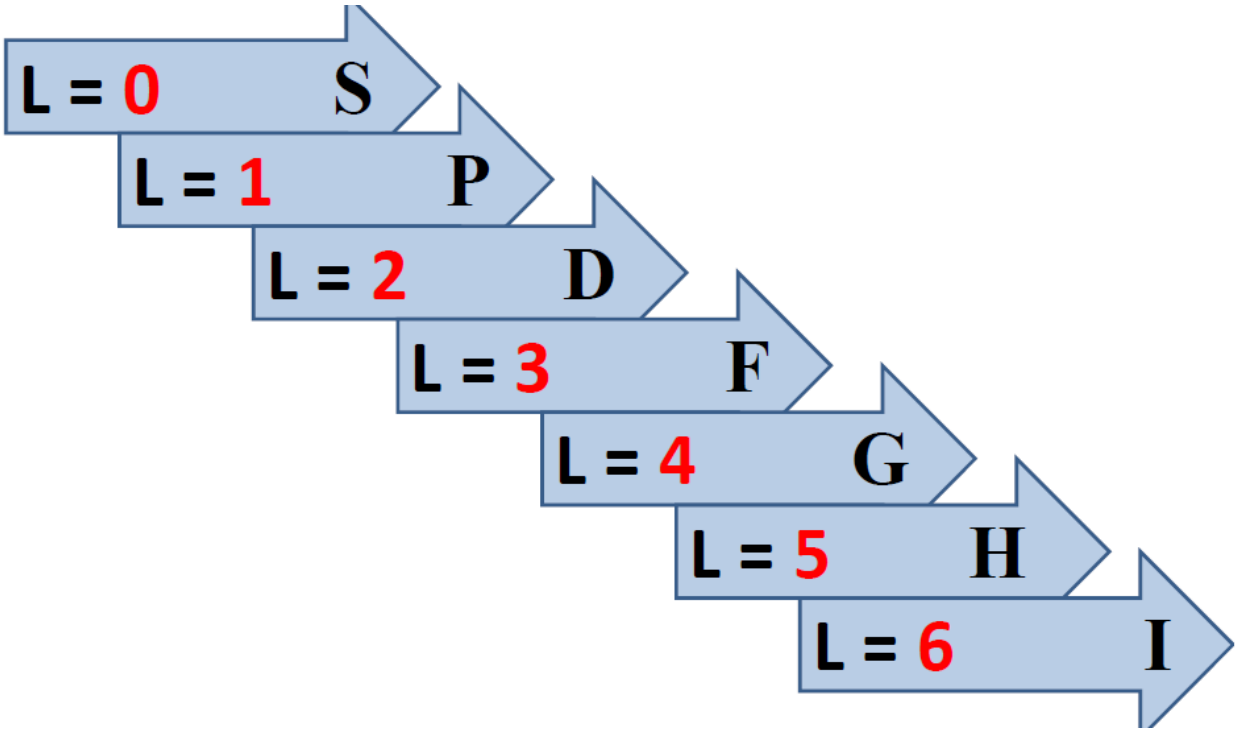
is used when the spin motion of the electron is coupled with the angular momentum of the orbital to a large degree. This method can be explained by saying that the angular momentum of the spin motion for each electron, then the values of j for the electron are coupled with the momentum of the orbital to give one value J for all electrons to give one value, which is J.

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

1- Electrons are distributed in orbitals of equal energy as much as possible, so that we can calculate the value of (S) to calculate the value of 2S+1, which is called the Bermi multiple.

2- Electrons take the orbitals that have the largest value for the number, then the next one, and so on, so that we get the largest value for the angular orbital momentum, L

(ml). Scientists have agreed to give capital letter values according to the following system:



3- If the number of electrons in the secondary orbital is:

J - more than half saturated, then we take the highest value for

J - less than half saturated, then we take the lowest value for

J - saturated or half saturated, then there is only one value for

$$J = /L+S/ \ldots\ldots\ldots\ldots /L-S/$$

To fined **Term symbol ($^{2S+1}L_J$) calculate:**

1) S

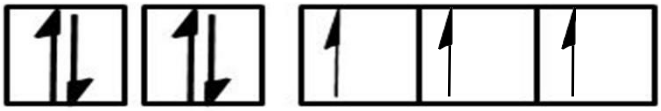
2) 2S+1

3) L

4) J

Example 1/ What is the symbol of the term in the stable state of nitrogen ($_7$N)?

$_7N :1S^2\ 2S^2\ 2P^3$



S = (+1/2) + (+1/2)+(+1/2)= 3/2

2S+1 =2× 3/2 + 1= 4

L = (+1) + (0)+(-1)= 0

J = /L+S/ ……/L-S/

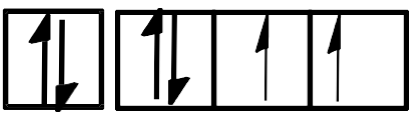
J = /0+3/2/ ……/0-3/2/= 3/2

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

$$^{4}S_{3/2}$$

Example 2/ What is the symbol of the term in the steady state of oxygen ($_8$O)?

$_8O :1S^2\ 2S^2\ 2P^4$



S = (+1/2)+(+1/2) = 1

2S+1 =2× 1 + 1= 3

L = (+1×2) + (0)+(-1)= 1

J = /L+S/ ……/L-S/

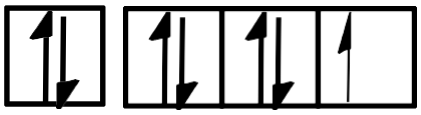
J = /1+1/ ……/1-1/= 2, 1, 0

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

$$^{3}P_2$$

Example 3/ What is the therm symbol in the stable state of a chlorine atom($_{17}$Cl)?

$_{17}Cl : 1S^2\ 2S^2\ 2P^6\ 3S^2\ 3P^5$



S = +1/2 = 1/2

2S+1 =2× 1/2 + 1= 2

L = (+1 ×2) + (0×2) + (-1×1) = 1

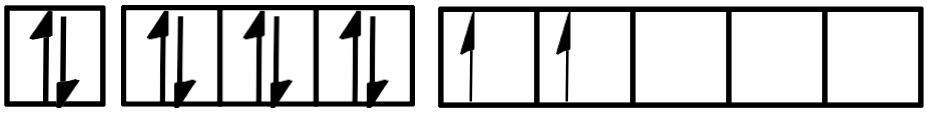
J = /1+1/2/ ……/1-1/2/= 3/2, …,1/2

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

$$^{2}P_{3/2}$$

Example 4/ What is the thermionic symbol in the stable state of the vanadium ion in the compound VF_3?

$_{23}V^{+3}$: $1S^2\ 2S^2\ 2P^6\ 3S^2\ 3P^6\ 4S^0\ 3d^2$



S = +1/2 +1/2 = 1

2S+1 =2× 1 + 1= 3

L = (+2× 1) + (+1 × 1) = 3

J = /L+S/ ……/L-S/

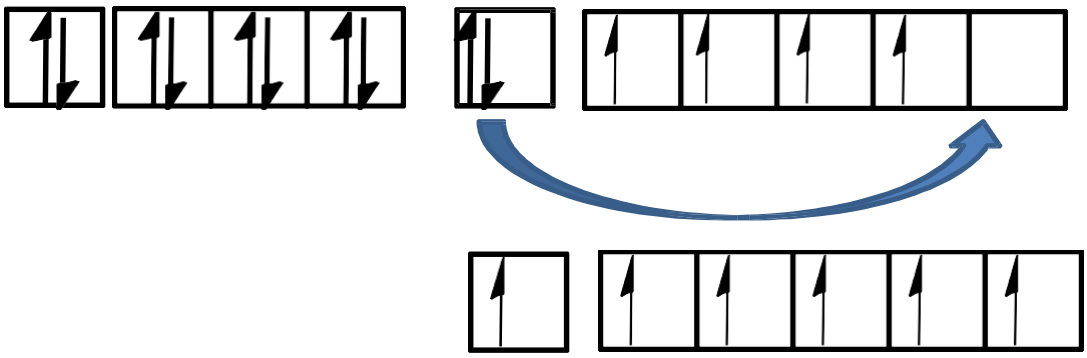
J = /3+1/ ……/3-1/= 4, 3, 2

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

$$^{3}F_2$$

Example 5/ What is the therm symbol in the stable state of the chromium atom($_{24}Cr$) ?

$_{24}Cr$:$1S^2\ 2S^2\ 2P^6\ 3S^2\ 3P^6$ $4S^2\ 3d^4$



S = +1/2 +1/2 +1/2 +1/2 +1/2 +1/2 = 3

2S+1 =2× 3 + 1= 7

L = ١ (+2) +١ (+1)+ 0 + ١(-2) +١ (-1) = 0

J = /0+3/ ……/0-3/= 3

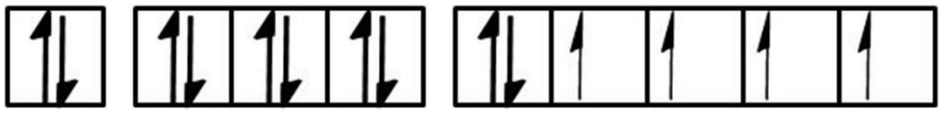
J = /L+S/ ……/L-S/

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

$$^{7}S_3$$

Example 6/ What is the term symbol in the steady state of the iron ion in the compound The atomic number of iron Fe = 26, O = 8?

$_{26}Fe^{+2}$:$1S^2$ $2S^2$ $2P^6$ $3S^2$ $3P^6$ $3d^6$



S = +1/2 +1/2 +1/2 +1/2 = 2

2S+1 =2× 2 + 1= 5

L = (+2×2) + (+1×1)+ 0 + (-1×1)+ (-2×1)= 2

J = /2+2/ ……/2-2/= 4, 3, 2, 1, 0

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

$$^{5}D_4$$

Question/ Find the term symbols for the stable state of the following atoms: (The solution is in parentheses, prove that it is correct)

1) $_{14}Si$ ($^3P_0$)

2) $_{22}Ti$ ($^3F_2$)

3) $_{27}Co$ ($^4F_{9/2}$)

4) $_{28}Ni$ ($^3F_4$)

5) $_{29}Cu$ ($^2S_{1/2}$)

Oxidation States:

An oxidation state, or oxidation number, is a number assigned to an element within a compound or molecule to represent how many electrons the element is capable of gaining or losing. Charge and formal charge are similar to the oxidation state, but these are different and separate concepts, even though the values tend to be the same in most cases. The following rules work for most compounds. If there is a conflict between two rules, always pick the rule that comes first.

1. An individual atom that is uncombined with any other element has an oxidation state of 0.

• O_2, N_2, H_2, C, and Ag would all have oxidation states of 0.

• The sum of the oxidation states of all the atoms in a compound must equal the charge.

• The oxidation state of a calcium ion (Ca^{+2}) would be +2.

• Since NaCl doesn't have a charge, the sum of the oxidation state for Na and Cl must be zero, so Na has a oxidation number of +1, while Cl has one of -1.

• In a compound, the oxidation state for Group 1 metals is +1 and Group 2 metals is +2.

• Sodium's oxidation state is +1 since it is a Group 1 metal.

• The oxidation state for F is -1 in a compound.

• The oxidation state for H is +1 in a compound.

• The oxidation state for O is -2 in a compound.

• In a two-element compound with metals, Group 15 elements will have an oxidation state of -3, Group 16 elements will have one of -2, and Group 17 elements will be -1.

• In HBr, H would have an oxidation state of +1 and Br would have an oxidation number of +1. For most compounds, you can immediately identify almost all of the elements' oxidation states; usually, you're left with one unknown oxidation state. In these cases, you would solve for the remaining oxidation number using Rule 2