**FACULTY OF SCIENCE, M.Sc ( CHEMISTRY ) , SEM- II , PAPER VII – CC VII**

**UNIT – I . ELECTRONIC SPECTRA OF TRANSITION METAL COMPLEXES**

**LECTURE No. 1- TERM SYMBOLS and SPIN ORBIT COUPLING**

**AUTHOR’S NAME - DR . A . KHAN**

**TERM SYMBOLS AND SPIN-ORBIT COUPLING (RUSSEL SAUNDER COUPLING)-**

This is also called as LS coupling scheme and it is appropriate for the first transition series ,the lanthanide series not too heavy atoms and ions.It is explored as under-

1. **COUPLING OF ORBITAL ANGULAR MOMENTUM**:

The all values or vectors of orbital angular momentum ( l- azimuthal quantum number ) of the electrons are couple together electrostatically to give the resultant vector L, called resultant orbital angular quantum number. Different values of L define the state of free atom or ion as a whole where as l define only the state of the electrons only.

1. The values of L are integers including zero and consider as different spectroscopic terms as given here

L = 0 = S , L = 1 =P , L = 2=D , L = 3 = F , L = 4 = G , L = 5 = H

The value of L for any filled orbitals ( s,p,d,f etc ) is taken zero.

1. **COUPLING OF SPIN ANGULAR MOMENTUM( S ):-**

All vectors of spin quantum number like l combine to give the resultant spin angular momentum number “ S “. It is an integer or half-integer depending on ther number of electrons and the direction of spin.

For ex- The spin value for two unpaired electron is + ½ for each ,hence the resultant value of S = (+1/2 ) + ( +1/2 ) = 1, and

For two paired electrons the resultant S = ( +1/2) + ( -1/2) = 0

The spin multiplicity = 2S + 1, called as spin multiplicity of L state.

1. **SPIN – ORBIT COUPLING OR L – S COUPLING( RUSSEL SAUNDER’S COUPLING).**

The resultant orbital angular quantum number”L” and resultant spin angular quantum number”S” further interact or couple together to give a new quantum number called as total angular momentum quantum number- J . This coupling is called Russel saunder coupling which is actually results from vectorial combination of L and S.

J = L + S = ( l1 + l­2 + l3 + ….. ) +  ( s 1 + s2 + …. ) = L + S

The values of J vary in between L + S and L – S ,so the J can have the following values

J = ( L + S ), ( L + S -1 ), ( L + S -2 )…………0, ( L – S +1 ), L – S

The term symbol of an atom oir ion is represented by - n + 1 L J

1. **DTERMINATION OF L VALUES FOR d n  CONFIGURATION / ( n - 1 ) d CONFIGURATION OF TRANSITION MATL ATOM / IONS**
2. **Rule I- a filled shell cannot contribute to the total** L and S so the value of both is zero.
3. **Rule II-**  The ground state is comprised of the highest value of spin multiplicity or which has the maximum number of unpaired electrons.
4. **Rule III-** For several number of terms with same spin multiplicity the term having the highest value of L treated as ground state term.
5. **Rule IV –**For a half filled or less than half filled, the ground state term is that which has the lowest value of J and for more than half filled, the ground state term is that which has the highest value of J.

**Thus the term symbol of atom or ion is written as** - n + 1 L J  or 2 S + 1 L J

|  |  |  |
| --- | --- | --- |
| SYSTEM | CONFIGURATIONS | RESULTANT L AND TERM SYMBOL |
| d1 & d9 | L= +2 +1 0 -1 -2   |  |  |  |  |  | | --- | --- | --- | --- | --- | | ˦ |  |  |  |  |  |  |  |  |  |  | | --- | --- | --- | --- | --- | | ˦ ˩ | ˦ ˩ | ˦ ˩ | ˦ ˩ | ˦ | | L = 2 = D or J = 5/2 , 3/2  Possible terms = 2D5/2, 2D3/2  **Ground state term for d1 =  2D3/2**  **Ground state term for d9 =  2D5/2** |
|  |  |  |
|  |  |  |
|  |  |  |
|  |  |  |
|  |  |  |
|  |  |  |