ATOMIC STRUCTURE

For
B.Sc-II Chemistry(H/S)
Inorganic Chemistry
Paper-III
Lecture-02

Estd.- 1962

By
Dr. Supriya kumari
J.L.N college,Dehri-on-Sone(Rohtas)
V.K.S.U,Ara
supriyachemu@gmail.com

ATOMIC STRUCTURE

Contets

- Heisenberg's Uncertainty Principle Equation
- Importace of Heisenberg's Uncertainty Principle
- Idea of group state terms symbol
- Excited state term symbol for d2 systum
- Term symbol for d^n configuration
- Groud Term symbol for d^n configuration

Atomic structure

Uncertainty principle:

- Introduced first in 1927, by the German physicist Werner Heisenberg
- The **uncertainty principle** states that the more precisely the position of some particle is determined, the less precisely its momentum can be predicted from initial conditions, and vice versa
- The position and the velocity of an object cannot both be measured exactly, at the same time, even in theory.

ATOMIC STRUCTURE

Importace of ucertainty principle:

The Heisenberg **uncertainty principle** is a law in quantum mechanics that limits how accurately you can measure two related variables. Specifically, it says that the more accurately you measure the momentum (or velocity) of a particle, the less accurately you can know its position, and vice versa.

Heisenberg's Uncertainty Principle Equation

Equation can be derived by assuming the particle of interest is behaving as a particle, and not as a wave. Simply let $\Delta p=mv$, and $\Delta x=h/(mv)$ (from De Broglie's expression for the wavelength of a particle).

What is the minimum uncertainty Δp in its momentum?

The **uncertainty** in position is the accuracy of the measurement, or $\Delta x = 0.0100$ nm.

Thus the smallest **uncertainty** in **momentum** Δp can be calculated using

$$\Delta x \Delta p \geq h/4\pi$$

and $\Delta x \, \Delta p \geq h/4\pi$

Once the **uncertainty** in **momentum** Δp is found, the **uncertainty** in velocity can be found from $\Delta p = m\Delta v$.

ATOMIC STRUCTURE

Idea of group state terms symbol

Term symbol

Hund's rule states that: Every orbital in a sublevel is singly occupied before any orbital is doubly occupied. All of the electrons in singly occupied orbitals have the same spin.

Rule to find the term symbol?

To calculate **the** maximum and minimum values and make intervening values separated by

1. **The term symbol** has **the** form $^{2S+1}L_J$.

this is 2S+1

The super-prefix is **the** spin multiplicity, for spin angular momentum S and L is the angular momentum

J symbol

In the Russell-Saunders coupling scheme, **term symbols** are in the form of $^{2S+1}L_J$, where S represents the total spin angular momentum, L specifies the total orbital angular momentum, and **J** refers to the total angular momentum.

ATOMIC STRUCTURE

electronic configuration symbols

The **term symbols** will be of the form 1P and 3P.

For the **1P** state, L=1 and S=0, so J=1.

For the second state **3P**, L=1 and S=1, so J=2,1,0.

Four microstates for this **configuration** with **term symbols** of **1P1 and 3P2, 3P1, and 3P0.**

l1=2 ml1=2,1,0,-1,-2 ms1=½, -½ l2=2

ml2=2,1,0,-1,-2 ms2=½, -½

The **ground state** of an atomic nucleus, atom, or molecule is its lowest energy **state**. Higher energy **states** are described as **excited states**. The **ground state** applies to any quantized property of a particle.

The **excited state** has one electron promoted

L is the total angular momentum for spectroscopic notation

L=0 1 2 3 4 ……..

S P D F G……..

S, P, D, F term is derived from the characteristics of the spectroscopic lines corresponding to orbitals **sharp, principal, diffuse, and fundamental**

Atomic structure

- The combination of an S value and an L value is called a **term**
- A combination of S, L and J is called a **level**.
- A given level has $(2J+1)$, which is the number of possible microstates associated with this level in the corresponding term.
- A combination of S, L, J and M_J determines a single **state**.
- (2S+1)(2L+1) gives possible number of microstates.

Atomic structure

Calculation of the term symbol for the ground state of an atom using Hund's rules.

- Start with the most stable electron configuration.
- Full shells and subshells do not contribute to the overall angular momentum .If all shells and subshells are full then the term symbol is $^1S_0$.
- Arrange the electrons in the **orbitals**, according to the Pauli exclusion principle.
- First, fill the orbitals with highest m_l value with one electron each, and assign a maximal m_s to them (i.e. +½). Once all orbitals in a subshell have one electron, add a second one (following the same order), assigning $m_s = -½$ to them.
- The overall *S* is calculated by adding the m_s values for each electron.
- According to Hund's first rule, the ground state has all unpaired electron spins parallel with the same value of m_s, conventionally chosen as +½. The overall *S* is then ½ times the number of **unpaired** electrons. The overall *L* is calculated by adding the m_l values for each electron.

Atomic structure

Excited state term symbol for d2 systum:

d^2

Example: free metal ion v^{+3}

L +2 +1 0 -1 -2

m_l +2 +1 0 -1 -2

m_s ↑ ↑

$S = ½ + ½ = 1$ and $L = 2 + 1 = 3$,

J = L+S ……to…… L-S

Here, J=3-1=2 less than half filled

S= 2s+1

2x1+1=3

so, term symbol for d^2

$^3F_2$

Ground state term symbol

^3F

Excited term symbol for d^2

^3P ^1G ^1D ^1S

Atomic structure

Configuration	Terms
d^1, d^9	^2D
d^2, d^8	^3F, ^3P, ^1G, ^1D, ^1S
d^3, d^7	^4F, ^4P, ^2H, ^2G, ^2F, ^2D (2), ^2P
d^4, d^6	^5D, ^3H, ^3G, ^3F (2), ^3D, ^3P (2), ^1I, ^1G (2), ^1F, ^1D (2), ^1S (2)
d^5	^6S, ^4G, ^4F, ^4D, ^4P, ^2I, ^2H, ^2G (2), ^2F (2), ^2D (3), ^2P, ^2S

Term symbol for d^n configuration

Atomic structure

Configuration	m_l 2	1	0	-1	-2	M_L	S	Ground term	Example
d^1	↑					2	1/2	^2D	Ti^{3+}
d^2	↑	↑				3	1	^3F	V^{3+}
d^3	↑	↑	↑			3	3/2	^4F	Cr^{3+}
d^4	↑	↑	↑	↑		2	2	^5D	Cr^{2+}
d^5	↑	↑	↑	↑	↑	0	5/2	^6S	Mn^{2+}
d^6	↑↓	↑	↑	↑	↑	2	2	^5D	Fe^{2+}
d^7	↑↓	↑↓	↑	↑	↑	3	3/2	^4F	Co^{2+}
d^8	↑↓	↑↓	↑↓	↑	↑	3	1	^3F	Ni^{2+}
d^9	↑↓	↑↓	↑↓	↑↓	↑	2	1/2	^2D	Cu^{2+}

Ground term for d^n configuration

Atomic structure

Problems for practice

Calculate and write the ground state terms for the following:

1. V^{+3}
2. Co^{+3}
3. Ti^{+3}
4. V^{+3}
5. Cr^{+3}
6. Cr^{+2}
7. Mn^{+2}
8. Fe^{+2}
9. Co^{+2}
10. Ni^{+2}