

Science of material

Material are of matter & matter are made up of Atoms

Rutherford's model

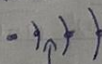
Quantum Atomic model base of The principle of Quantum mechanism.

Quantum mechanism:-

Quantum is a packet of Energy
Atomic radius of Atom is $\approx 10^{-10}$ m
 $1.0 \times 10^{-10} \approx 1.99999 \times 10^{-10}$

Quantum mechanism is base of

1. Quantization of energy, Which say energy is neither gain nor loss in a Continuous manner but in discrete packet Called quantum.


prohibited zone

$$E = -\frac{13.6}{n^2} \quad , \quad h = \text{Energy (electron volt)}$$

$n = \text{principal number}$

Energy between 2 orbit give us A quantum

$$E_1 = \frac{-k}{1^2} = -k$$

$$E_2 = \frac{-k}{2^2} = -\frac{k}{4}$$

$$E_3 = \frac{-k}{3^2} = -\frac{k}{9}$$

First quantum

$$E_2 - E_1 = -\frac{k}{4} - (-k)$$

$$= -\frac{k}{4} + k$$

$$= \frac{3}{4}k$$

Second quantum

$$E_3 - E_2 = \frac{-k}{9} - \left(-\frac{k}{4}\right) = -\frac{k}{9} + \frac{k}{4} = \frac{5}{36}k$$

$$E_{11} - E_{10} = \frac{-k}{(11)^2} - \frac{-k}{(10)^2}$$

$$= \frac{k}{10^2} - \frac{k}{11^2} = \frac{21}{12100}k$$

$$1.736 \times 10^{-3} k$$

$$E_{101} - E_{100} = \frac{k}{(100)^2} - \frac{k}{(101)^2} = 1.97 \times 10^{-6}$$

$$E_{1001} - E_{1000} = \frac{k}{(1000)^2} - \frac{k}{(1001)^2} = 1.997 \times 10^{-9}$$

Pauli Exclusion Principle

States that no 2 electrons in an atom can have the same set of quantum numbers. or no more than 2 electrons can occupy the same orbital in an atom. An orbital is a space within an atom where the probability of finding an electron is not equal to zero.

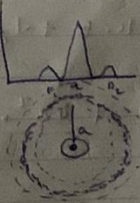
Heisenberg Uncertainty principle states that no 2 parameter describing the motion of an electron can be measured simultaneously with unlimited accuracy.

$$\Delta p \Delta x \geq \frac{h}{2\pi}$$

$$\Delta E \Delta t \geq \frac{h}{2\pi}$$

p = momentum, x = position, E = energy
 t = time

probability graph



Wave mechanics

De broglie postulate wave mechanics

$$\lambda = \frac{h}{p}$$

Le Schrodinger Postulation ~~that~~ a linear partial equation that govern the wave function of a quantum mechanical system.

$$\frac{d^2 A}{dx^2} + \frac{4\pi^2 A}{\lambda^2} = 0$$

$$\frac{d^2 \psi}{dx^2} + \frac{4\pi^2 \psi}{\lambda^2} = 0$$

$$\frac{d^2 \psi}{dx^2} + \frac{4\pi^2 p^2 \psi}{h^2}$$

$$\lambda = \frac{h}{p}, \quad p = mv, \quad p^2 = m^2 v^2 = 2m \left(\frac{1}{2} m v^2 \right)$$

$$\frac{1}{2} m v^2 = K.E$$

$$E = K.E + V, \quad K.E = E - V$$

$$\frac{d^2 \psi}{dx^2} + \frac{4\pi^2 \cdot 2m (E - V) \psi}{h^2} = 0$$

$$\left[\nabla^2 + \frac{4\pi^2 2M (E - V) \psi}{h^2} = 0 \right] \begin{array}{l} \text{3 dimensional} \\ \text{Schrödinger} \\ \text{equation.} \end{array}$$

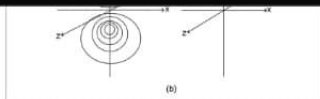


Fig. 1.38 (a) Wave functions ψ for s, p and d atomic orbitals. (Note that the + and - signs refer to symmetry, not charge.) (b) Different ways of representing ψ^2 for a 2p orbital (as a contour diagram or as a 90% boundary surface)

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Hence the probability of finding the electron ψ^2 , depends only on the distance r from the nucleus, and is the same in all directions.

$$\psi = f(r).$$

This leads to a spherical orbital, and occurs when the subsidiary quantum number l is zero. These are called s orbitals. When $l = 0$, the magnetic quantum number $m = 0$, so there is only one such orbital for each value of n .

In the second group of solutions to the wave equation, ψ depends both on the distance from the nucleus, and on the direction in space (x , y or z). Orbitals of this kind occur when the subsidiary quantum number $l = 1$. These are called p orbitals and there are three possible values of the magnetic quantum number ($m = -1, 0$ and $+1$). There are therefore three orbitals which are identical in energy,

Atomic Structure 1.59

shape and size, which differ only in their direction in space. These three solutions to the wave equation may be written

$$\psi_x = f(r) \cdot f(x)$$

$$\psi_y = f(r) \cdot f(y)$$

$$\psi_z = f(r) \cdot f(z)$$

Orbitals that are identical in energy are termed degenerate, and thus three degenerate p orbitals occur for each of the values of $n = 2, 3, 4, \dots$

Principal quantum number n	Subsidiary quantum number l	Magnetic quantum numbers m	Symbol
1	0	0	
2	0	0	
2	1	-1, 0, +1	
3	0	0	
3	1	-1, 0, +1	
3	2	-2, -1, 0, +1, +2	
4	0	0	
4	1	-1, 0, +1	
4	2	-2, -1, 0, +1, +2	
4	3	-3, -2, -1, 0, +1, +2, +3	

The third group of solutions to the wave equation depend on the distance from the nucleus r and also on two directions in space, for example,

$$\psi = f(r) \cdot f(x) \cdot f(y)$$

This group of orbitals has $l = 2$, and these are called d orbitals. There are five solutions corresponding to $m = -2, -1, 0, +1$ and $+2$, and these are all equal in energy. Thus five degenerate d orbitals occur for each of the values of $n = 3, 4, 5, \dots$

A further set of solutions occurs when $l = 3$, and these are called f orbitals. There are seven values of m , $-3, -2, -1, 0, +1, +2$ and $+3$, and seven degenerate f orbitals are formed when $n = 4, 5, 6, \dots$



Worked-out Examples

47. The electrons, identified by quantum numbers n and l , (i) $n = 4, l = 1$, (ii) $n = 4, l = 0$, (iii) $n = 3, l = 2$, and (iv) $n = 3, l = 1$ can be placed in order of increasing energy, from the lowest to highest, as [IIT-1999]

(a) (iv) < (ii) < (iii) < (i)

(b) (ii) < (iv) < (i) < (iii)

(c) (i) < (iii) < (ii) < (iv)

(d) (iii) < (i) < (iv) < (ii)

Solution. (a) The two guiding rules to arrange the various orbitals in the increasing energy are:

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(d) $\uparrow\downarrow \uparrow\downarrow \downarrow \downarrow \downarrow$

Solution (a, d) Only the configurations (a) and (d) follow Hund's rule.

THE SCRODINGER WAVE EQUATION

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For a standing wave of wavelength λ , whose amplitude at any point along x may be described by a function $f(x)$, it can be written that

$$\frac{d^2 f(x)}{dx^2} = -\frac{4\pi^2}{\lambda^2} f(x)$$

If an electron is considered as a wave which moves in only one dimension then

$$\frac{d^2 \psi}{dx^2} = -\frac{4\pi^2}{\lambda^2} \psi$$

An electron may move in three directions x , y and z so this becomes

$$\frac{\partial^2 \psi}{\partial x^2} + \frac{\partial^2 \psi}{\partial y^2} + \frac{\partial^2 \psi}{\partial z^2} = -\frac{4\pi^2}{\lambda^2} \psi$$

Using the symbol ∇ instead of the three partial differentials, this can be shortened to

$$\nabla^2 \psi = -\frac{4\pi^2}{\lambda^2} \psi$$

Atomic Structure 1.57

The de Broglie relationship states that,

$$\lambda = \frac{h}{mv}$$

(where h is Planck's constant, m is the mass of an electron and v its velocity); hence,

$$\nabla^2 \psi = \frac{4\pi^2 m^2 v^2}{h^2} \psi$$

or

$$\nabla^2 \psi + \frac{4\pi^2 m^2 v^2}{h^2} \psi = 0 \quad (i)$$

However, the total energy of the system E is made up of the kinetic energy K plus the potential energy V

$$E = K + V$$

so

$$K = E - V$$

But the kinetic energy $= \frac{1}{2} mv^2$

Therefore, $\frac{1}{2} mv^2 = E - V$

$$v^2 = \frac{2}{m} (E - V)$$

Substituting for v^2 in equation (i) gives the well-known form of the Schrodinger equation

$$\nabla^2 \psi + \frac{8\pi^2 m}{h^2} (E - V) \psi = 0$$

Acceptable solutions to the wave equation, that is solutions which are physically possible, when ψ is finite, continuous, single valued and

- The probability of finding the electron over all the spaces from plus infinity to minus infinity must be equal to one.

The probability of finding an electron at a point x, y, z is ψ^2 , so,

$$\int_{-\infty}^{+\infty} \psi^2 dx dy dz = 1$$

Several wave functions called $\psi_1, \psi_2, \psi_3, \dots$ will satisfy these conditions to the wave equation.



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