# Quadrant II – Transcript and Related Materials

**Programme:Bachelor of Science (First Year)**

**Subject: Chemistry**

**Paper Code: CHC 101**

**Paper Title: Inorganic Chemistry and Organic Chemistry (Section A)**

**Unit: 1**

**Module Name:Radial distribution functions and the concept of the most probable distance with special reference to 1s and 2s atomic orbitals.**

**Module No: 10**

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## Notes

Radial distribution curves for 1s and 2s atomic orbitals from radial wave function shall help to understand the most probable distance of an electron in 1s and 2s atomic orbitals.

Consider the time-independent form of the Schrodinger wave equation.

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

-----------eq1

Above Schrodinger wave equation represents the wave in three dimensions x, y, z (Cartesian coordinates). As a point in space can be defined using polar coordinated we can substitute the polar coordinates R, $\theta$ and $\phi$ in the Schrodinger equation. We can also substitute mass m by the reduced mass $\mu$. The new form of the Schrodinger equation is as follows.

$$\frac{1}{r^2}\frac{d}{dr}(r^2\frac{d\psi}{dr})+\frac{1}{r^2\sin\theta}\frac{d}{d\theta}(\sin\theta\frac{d\psi}{d\theta})+\frac{1}{r^2\sin^2\theta}\frac{d^2\psi^2}{d\phi^2}+\frac{8\pi^2\mu}{h^2}(E-V)=0$$

-----------eq2

From eq2 it is evident that the Schrodinger wave equation has a component that is dependent on the radius (a radial component of a wave function) and there is an angular component dependent on $\theta$and $\phi$.

Thus eq2 can be written as

$$\boldsymbol{\psi(r, \theta, \phi) = R(r), \Theta(\theta), \Phi(\phi)}$$

-----------eq3

Radial component 'R(r)' of wave function '**ψ**' gives the distribution of electron as a function of the radius that is the distance from the nucleus 'r'

The radial wave function depends on principle quantum number 'n' and azimuthal quantum number 'l' and has a common function

$$\boldsymbol{e^{-Zr/na_\circ}}$$

-----------eq4

Where,

r = distance from nucleus

e = base of the natural logarithm

Z = atomic number

a°= Bohr radius (52.9 pm)

n = principal quantum number

To understand the most probable distance of an electron in 1 s and 2 s atomic orbitals we can consider H atom which has only one electron and the atomic number is 1.

Table 1.Mathematical expression of Radial wave function '**R(r)**' for 1s and 2s orbital

| Orbital | Quantum number | Radial wave function '**R(r)**' |
|---|---|---|
| 1s | n = 1, l = 0 | $2(\frac{Z}{a_\circ})^{3/2}e^{-Zr/na_\circ}$ |
| 2s | n = 2, l = 0 | $\frac{1}{8^{\frac{1}{2}}}\left(\frac{Z}{a_\circ}\right)^{\frac{3}{2}}\left(2-\frac{2Zr}{\mathrm{n}a_\circ}\right)e^{-Zr/na_\circ}$ |

The radial wave equations (Table 1) have no physical significance but a plot of a square of radial function‘$[R(r)]^2$’which is also called radial distribution function, gives the probability of finding an electron at a fixed distance in space around the nucleus.

The H atom where Z=1, for the 1s orbital electron plot the radial wave function in two-dimensional space and we observe a curve (Figure 1) plot of radial distribution function (Figure 2)appears asa Gaussian curve. If we observe the value of the radial distribution function at which this radial distribution function values are maximum we arrive at a value of 52.9 pm. This is the most probable distance of the 1s electron.

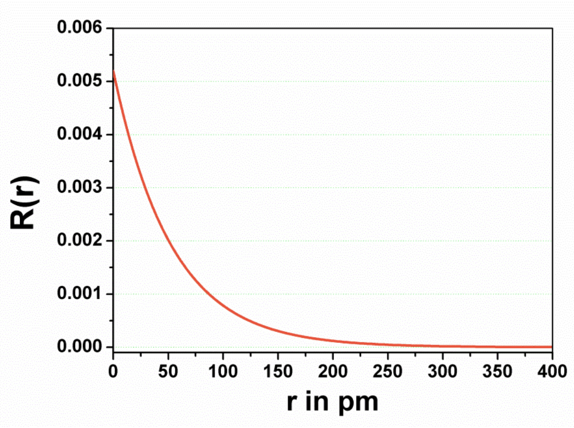

Figure 1.Radial wave function of 1s orbital.

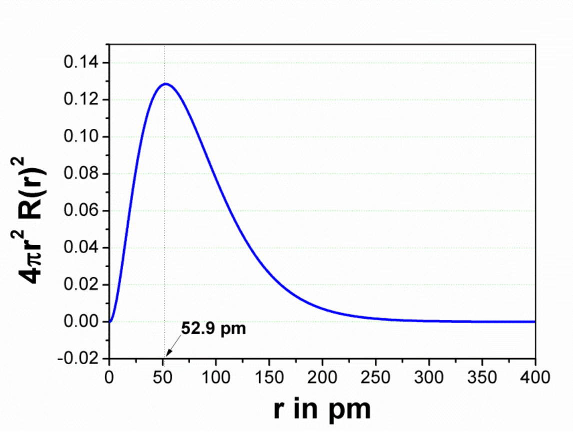

Figure 2. Radial distribution function of 1s orbital.

Theoretically, we can elaborate it for 2s electron of H atom although there is no 2s electron in H atom. The plot of a radial wave function(Figure 3) for 2s is a wavy curve. There is a particular point at which this value of radial wave function is zero this means the square of this value will be zero and the probability of finding an electron is zero at this point(Figure 4). This point is called a node and it is a radial node. The probability function is highest at around 300 pm. That is the distance at which the ismaximum chance of finding the 2s electron.

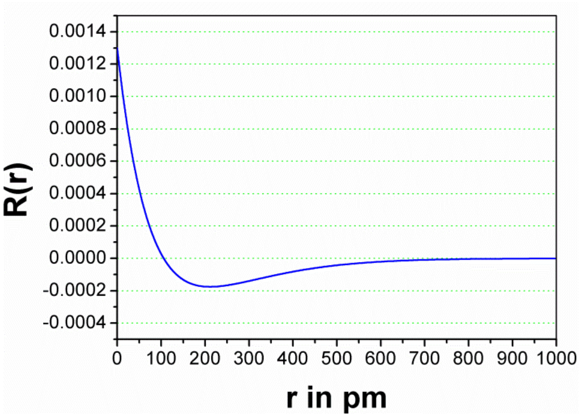

Figure 3.Radial wave function of 2s orbital.

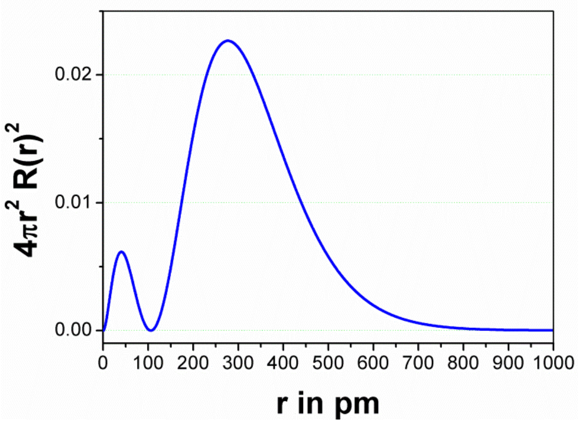

Figure 4.Radial distribution function of 2s orbital.

The probability of finding 1s electrons is closer to the nucleus than 2s electrons. There are no radial nodes in 1s orbital and one radial node in 2s orbital.