

Welcome students for FY Inorganic Chemistry section A.

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So today we're going to take up the module: radial and angular nodes from unit Atomic Structure.

So outline of this module: We are going to 1st see the definition of node. Then, what are radial and angular wave functions? What are angular and radial nodes? Then, the significance of these nodes and finally will try to calculate these nodes and find the size and shape of the orbitals.

Learning outcomes: At the end of this module, we will be having an understanding of orbital and node in an atom. Will know about the radial and angular component of wave function and finally will be able to calculate the total number of nodes with corresponding radial and angular nodes for different orbitals.

So let's start. So, first is what are nodes? So nodes are defined as the region at which the probability of finding an electron is zero. So this is how an atomic structure you have learned to draw with nucleus at the center and around the nucleus, we have the concentric circles which represents the shells or the orbits, and these orbits are designated as K, L, M, N and these orbits have further orbitals. So, K orbit has 1s; L has 2s and 2p orbitals and so on. Now in the textbooks, you will see that orbits and orbitals are used interchangeably, so both are correct. So you can at times call these orbits as orbitals as well. Now further you had learned that between these concentric circles, the space which is there is denoted as nodes. And you have to remember here that nucleus is not considered as a node. Now, in this module we're going to focus basically on the node and these nodes which are further of two types: Radial node and Angular node.

So then in the previous module you have learned how to represent the orbital in terms of wave function i.e. given by  $\psi_{n,l,m} = R_{n,l}(r) Y_{l,m}(\theta, \phi)$ . The subscripts n, l & m are the quantum numbers and in the brackets what you have are (Theta and phi) are the polar coordinates. These polar coordinates tells the position of the electrons in an orbital in 3 dimensional space. Next in this Equation the R component over here represents the radial wavefunction and Y represents the angular wavefunction. Here, radial wavefunction gives the size of the orbital whereas the Y component gives the shape of the orbital.

Now, we also know that the value of  $\psi^2$  gives the electron density distribution. And when the  $\psi^2$  reaches to zero, we get the node. That means when either R component or Y component or both of them have zero value, automatically we get  $\psi^2$  value as zero. So one representative graph I have put over here wherein you can see when a  $\psi^2$  is plotted with respect to radius. The two humps represents the two orbitals that is 1s orbital and 2s orbital and the depression over there where  $\psi^2$  reaches to zero is the node. And that is what we are going to learn in this module.

Now quickly will see the dependence of orbitals on the polar coordinates i.e., r, theta, and phi. Over here, 'r' represents the radius and theta & phi represents the angles. Here, the radial part of the wavefunction is always positive value. It is because radius has to be a positive value. The angular part of the wave

function may be positive or negative as it depends on the two angles, i.e.  $\theta$  and  $\phi$ . So, we have learned that *s*-orbital has a circular shape as it is only dependent on radius and not on the angles and that has positive value and the *p*-orbital is represented by a dumbbell shape which has one lobe as positive and the other lobe as negative and the *d*-orbital which is represented by double dumbbell shape. The *d*-orbital angular dependence gives the opposite lobes with identical sign.

Now coming to what are radial nodes and angular nodes? First radial nodes. Radial nodes occur where the radial component that is  $R$  of the wave function passes through zero means the probability of finding electron over here becomes zero. Now these regions are described as radial nodes or spherical radial nodes as they have fixed radius and depicts the size and are circular in shape. And the number of radial nodes are determined from the principle quantum number that is ' $n$ '.

Coming to Angular nodes, angular nodes occur when angular component  $Y$  of the wave function passes through zero. Now these regions are described as angular nodes, nodal planes or it can be conical as well and they have fixed angles as the  $Y$  component depends on the angle  $\theta$  &  $\phi$ . The number of angular nodes is determined by azimuthal quantum number that is ' $l$ '.

Now, the significance of these radial or angular nodes: now radial wavefunction gives the size of the orbital. The number of radial node increases as the number of principle quantum number ' $n$ ' increases and the angular part of the term determines its shape. Angular node is equal to azimuthal quantum number ' $l$ '. From the value of  $m$  &  $l$ , the number of nodes is derived and the type of node is determined.

Now quickly we'll see how to calculate these nodes. So these are the formulas. So total number of nodes is found out from the principle quantum number that is ' $n$ ', it is  $n - 1$ . The angular nodes is equal to the value of ' $l$ '. And for the number of radial nodes, we have two formulas, one is (the number of nodes - angular nodes) that is  $(n - 1 - l)$ . And the other formula is with respect to which orbital it belongs to. So if it is *ns* it is going to be  $n - 1$  and for *np* it will be  $n - 2$  and so on.

We will calculate for some of the orbitals, so first we'll see for the first shell or the first orbit, having one *s*-orbital. So the value of ' $n$ ' is 1 and the value of ' $l$ ' is 0. So I've shown here, how to know the value of  $n$  &  $l$ , so one which is the number represents the principle quantum number  $n$  and  $s$  represents ' $l$ ' and depending on this alphabet the value of ' $l$ ' is given. So for 1*s*,  $n$  has to be 1 and  $l = 0$  and so on. So now let's calculate the number of nodes for it. So it's going to be  $n - 1$ , that is  $1 - 1 = 0$ . The angular nodes is just the number of the value of  $l$  that is 0. Then the number of radial nodes with both the methods, we get it as zero. So in total the type of nodes or the total number of nodes is 0. So you can see over here 1*s* orbital does not have any orbital. I'll repeat over here that nucleus is not considered as a node. So 1*s* orbital does not have any node. So you have shown a planar structure. Just remember this is a three dimensional structure, so you can imagine a tennis ball. So inside you have a nucleus and the surface it is all 1*s* orbital.

Now coming to the next shell i.e., second shell which has 2*s* and 2*p* orbital. So you get number of nodes as 1, angular nodes zero and radial nodes as one. So 2*s* orbital has one radial node and similar

calculations for 2p, we will get number of nodes as one and angular nodes one and radial nodes are zero. So your total number of nodes is 1 and the type of node is angular node. So here is one of the representation figure, where you can see for 2s orbital you have 1s and then you have the one radial node and then 2s orbital. So one of the two  $p_x$  orbital I've shown over here, you can see this is the angular plane, that is nodal plane, passing through the nucleus and dividing the two lobes. Similarly, calculating for the third shell having 3s, 3p and 3d orbital, you can see number of nodes comes to 2 and for 3s orbital, you get 2 radial nodes, for 3p orbital, one radial and one angular node. And for 3d you have two angular nodes. OK, so you have to remember the total number of nodes. It can be both or all of them can be radial, all of them can be angular or it can be radial + angular.

so now you can see in 3s orbital as I had said as the principle number increases your number of radial nodes also increases, right? So you have two radial nodes for this. For 3s, you can see a plane and a radial node over here. In 3p we can see two planes. And for 3d, one cone.

So to summarize, the nodes are the points/planes of zero electron density. Radial nodes determines the size and they're spherical in shape, whereas angular nodes determines the shape of the orbital and they're planar or conical.

These are the references for some standard books. They are Puri & Sharma, Huyee, J.D Lee, etc.

Thank you.