## ❖ Shape of Atomic Orbitals (*s*, *p* & *d*)

The wave mechanical model of atom says that there is a non-zero probability of finding the electron almost everywhere in space excepting the angular and radial nodes. This means that primitive diagrams that depict the orbital shapes are intended to describe the region encompassing 90−95% probability density. In a typical drawing of orbital, we first plot the radial wave function and the angular part is superimposed. The shapes of some typical orbitals are discussed below.

### ➢ *Shape of s-Orbitals*

In order to draw the shape of s-orbital, we first need to recall the radial part of the same and then we will have to superimpose the angular part. For instance, the radial part of 1*s* orbital is

$$R_{1,0} = 2\left(\frac{1}{a_0}\right)^{3/2} e^{-r/a_0} \tag{443}$$

It is obvious from the equation (443) that the radial part of the wave function has the largest magnitude when $r = 0$, and it decreases as we move away from the nucleus. The function will become zero only at infinite distance and will never change its sign. All this leads to a spherical-shaped cloud without any radial node. The angular part of every *s*-orbital is

$$Y_{0,0} = \frac{1}{\sqrt{4\pi}} = 0.28 \tag{444}$$

Hence, after multiplying radial wave function by a constant value of the angular part, the magnitude of function at all the points in space will reduce to 28% of the initial value.

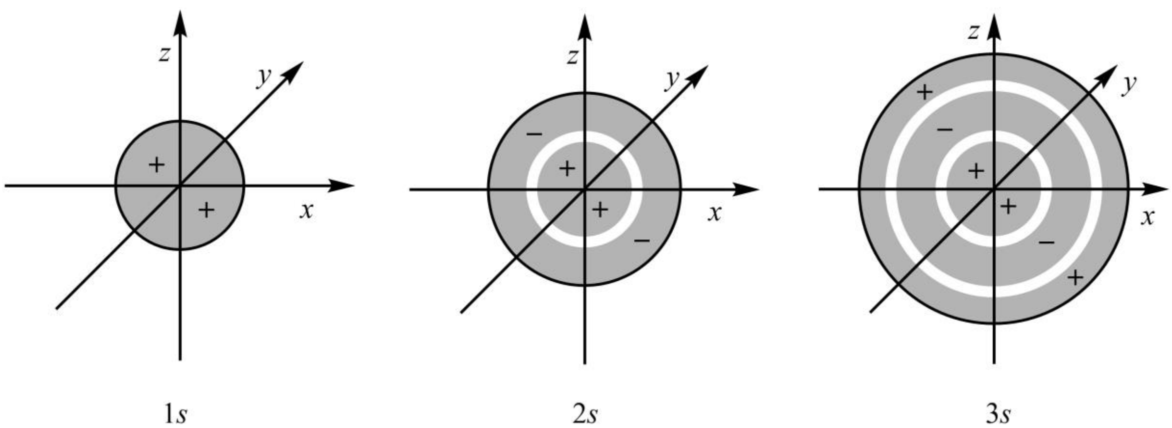


Figure 26. The shape of some lower energy *s*-orbitals.

Similarly, the shapes of some other s-orbitals are also given below to explain the concept more precisely. It is worthy to mention that the plots are easy to draw if we treat radial and angular parts consequently.

### ➢ *Shape of p-Orbitals*

In order to draw the shape of *p*-orbital, we first need to recall the radial part of the same and then we will have to superimpose the angular part. For instance, the radial part of 2*p* orbital is

$$R_{2,1} = \frac{1}{2\sqrt{6}}\left(\frac{1}{a_0}\right)^{3/2}\left(\frac{r}{a_0}\right)e^{-r/2a_0} \tag{445}$$

It is obvious from the equation (445) that the radial part of the wave function has the zero magnitudes when $r = 0$; and it increases as we move away from the nucleus, reaches a maximum, and decreases afterward. The function becomes zero only at infinite distance and will never change its sign. All this leads to a spherical-shaped cloud without any radial node. The angular part of *p*-orbitals are

$$Y_{1,0} = \sqrt{\frac{3}{2}}\,Cos\,\theta.\frac{1}{\sqrt{2\pi}} \tag{446}$$

$$Y_{1,\pm1} = \sqrt{\frac{3}{2}}\,Sin\,\theta.\sqrt{\frac{1}{2\pi}}\,e^{\pm i\phi} \tag{447}$$



Hence, the full plot for $p_z$-orbital is obtained after multiplying radial wave function by angular part given by equation (446); and the sign of function above the *xy*-plane will remain positive whereas a negative sign will be obtained below *xy*-plane. Similarly, we can obtain the three-dimensional plots for $p_x$ and $p_y$ by multiplying equation (445) by equation (447).

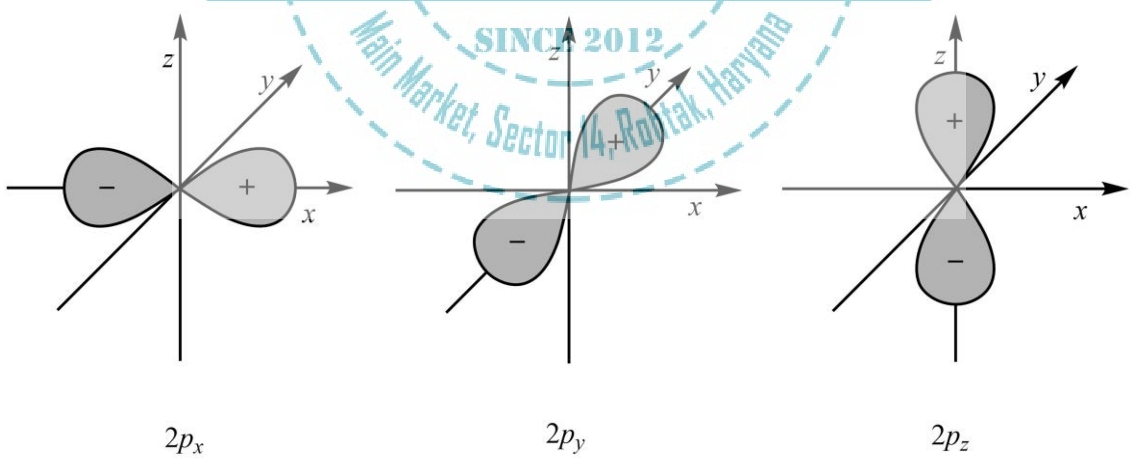


Figure 27. The shape of 2*p*-orbitals.

Similarly, the shapes of some other *p*-orbitals are also given below to explain the concept more precisely. It is worthy to mention that the plots are easy to draw if we treat radial and angular parts consequently.

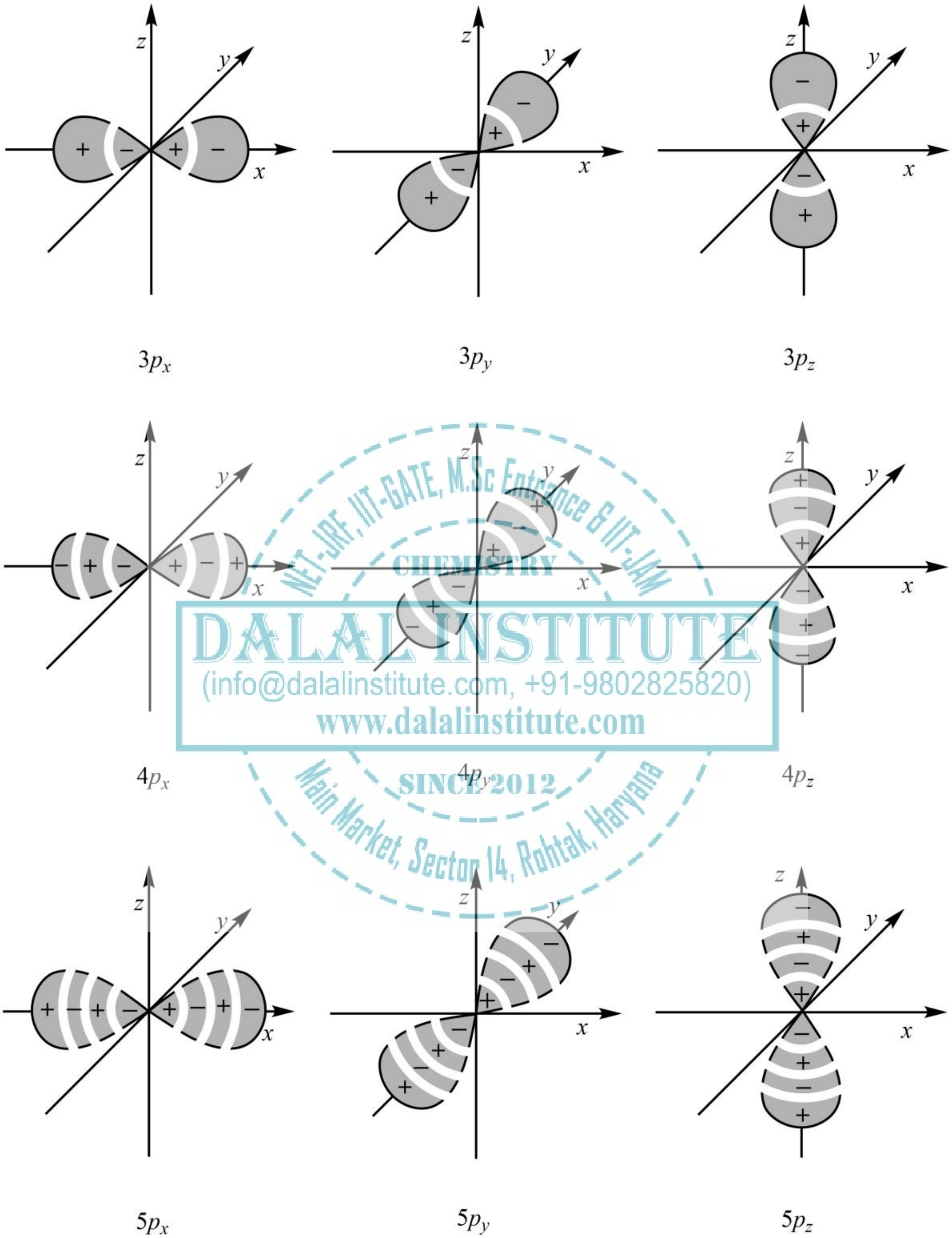




Figure 28. The shape of some 3*p*, 4*p* and 5*p* orbitals.

### ➢ ***Shape of d-Orbitals***

In order to draw the shape of *d*-orbital, we first need to recall the radial part of the same and then we will have to superimpose the angular part. For instance, the radial part of 3*d* orbital is

$$R_{3,2} = \frac{1}{81\sqrt{30}}\left(\frac{Z}{a_0}\right)^{3/2}\left(\frac{Zr}{a_0}\right)^{3/2} - \left(\frac{Zr}{a_0}\right)^{2} e^{-Zr/3a_0} \tag{448}$$

It is obvious from the equation (448) that the radial part of the wave function has the zero magnitudes when $r = 0$; and it increases as we move away from the nucleus, reaches a maximum, and decreases afterward. The function becomes zero only at infinite distance and will never change its sign. All this leads to a spherical-shaped cloud without any radial node. The angular part of *d*-orbitals are

$$Y_{2,0} = \sqrt{\frac{5}{8}}(3Cos^2\,\theta - 1).\frac{1}{\sqrt{2\pi}} \tag{449}$$

$$Y_{2,\pm 1} = \sqrt{\frac{15}{4}}\,Sin\,\theta\,Cos\,\theta.\sqrt{\frac{1}{2\pi}}e^{\pm i\phi} \tag{450}$$

$$Y_{2,\pm 2} = \sqrt{\frac{15}{16}}\,Sin^2\,\theta.\sqrt{\frac{1}{2\pi}}e^{\pm i2\phi} \tag{451}$$

Hence, the full plot for $d_{z^2}$-orbital is obtained after multiplying radial wave function by angular part given by equation (449); and the sign of function in the *xy*-plane will become negative whereas a positive sign will be obtained in two opposite lobes along *z*-axis. It is also worthy to note that the function becomes completely zero in two conical surfaces (above and below) before changing its sign. Similarly, we can obtain the three-dimensional plots for $p_x$ and $p_y$ by multiplying equation (448) by equation (450, 451).

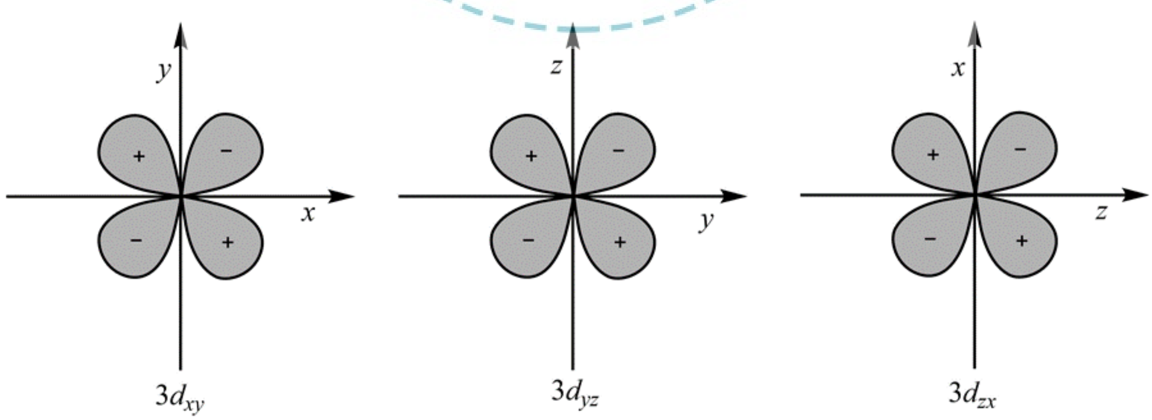


*Figure 29. Continued on the next page…*

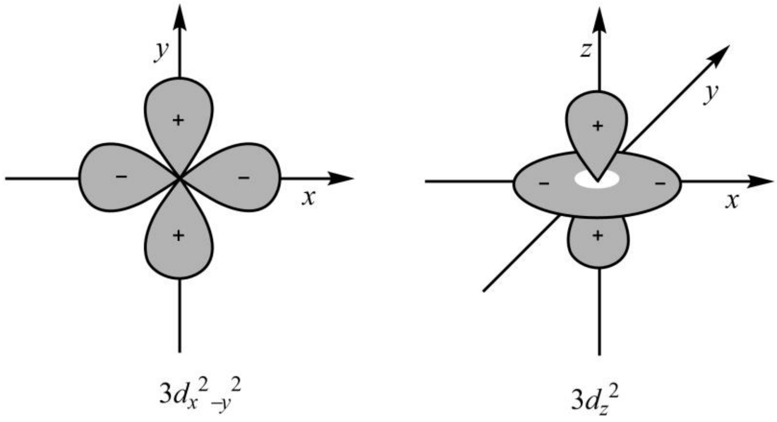


Figure 29. The shape of 3$d$-orbitals.

Similarly, the shapes of some other $d$-orbitals are also given below to explain the concept more precisely. It is worthy to mention that the plots are easy to draw if we treat radial and angular parts consequently.

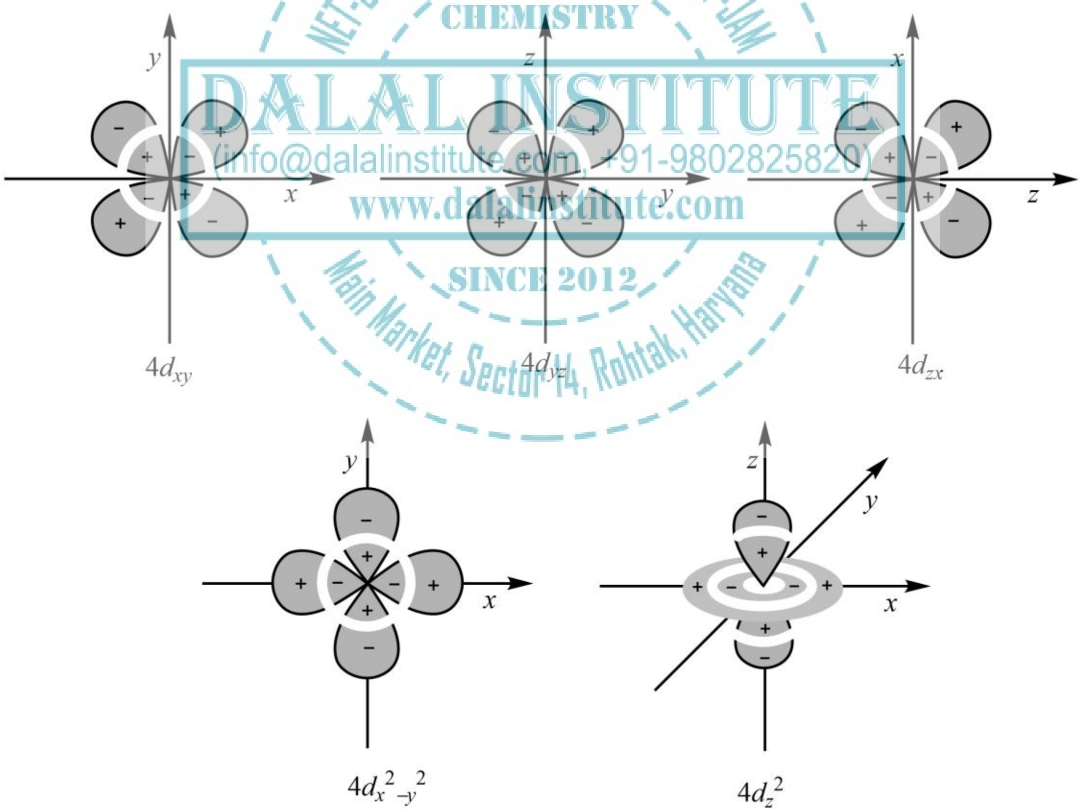


Figure 30. The shape of 4$d$ orbitals.

It is also worthy to mention that the radii of maximum probability for 4*d* orbitals are larger than that of 3*d* orbitals. The same is true for *s* and *p* orbitals i.e. radius of maximum probability of *s* and *p* orbitals follow the order 3*s* > 2*s* > 1*s* and 4*p* > 3*p* > 2*p*, respectively.

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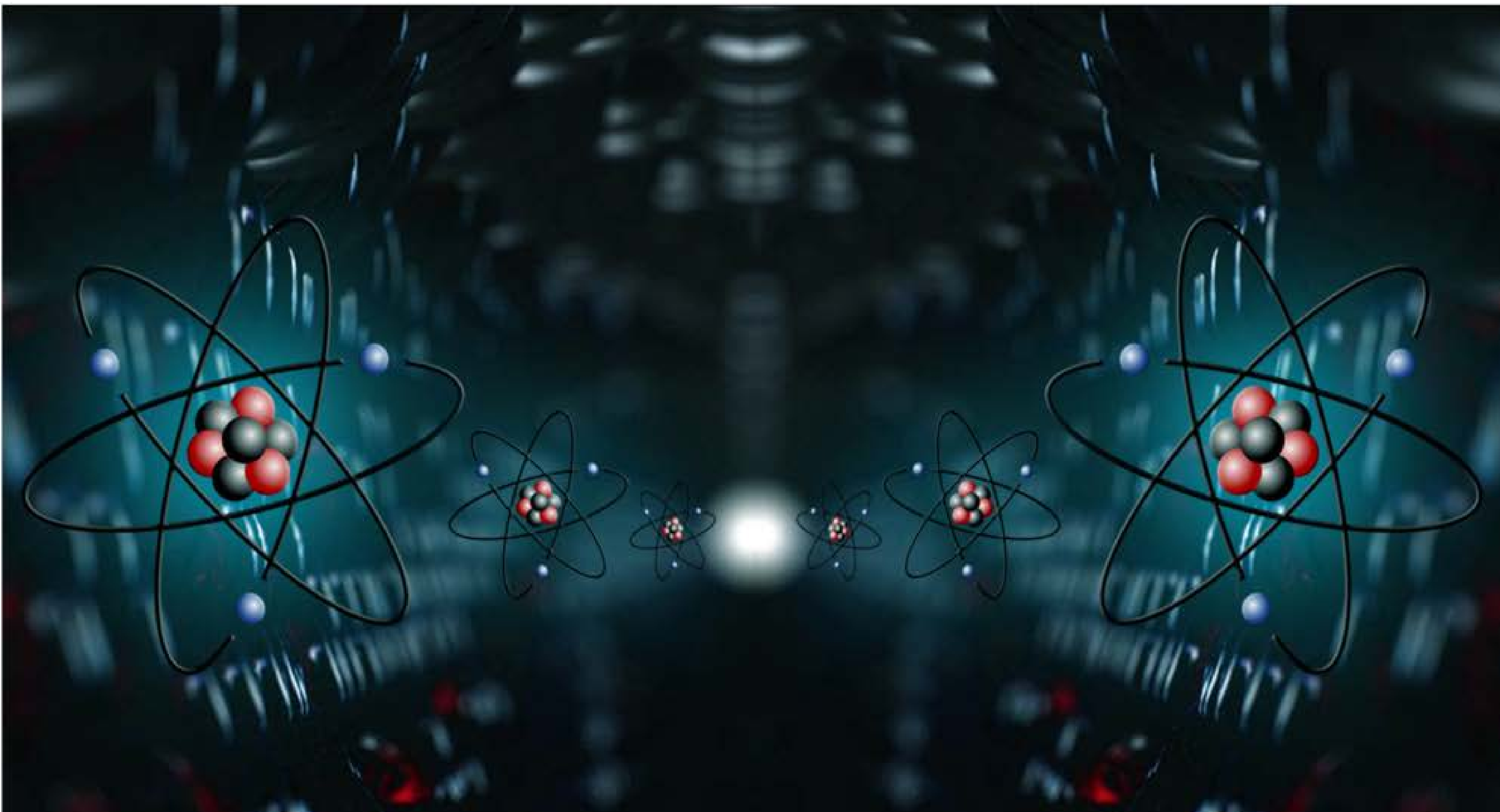

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