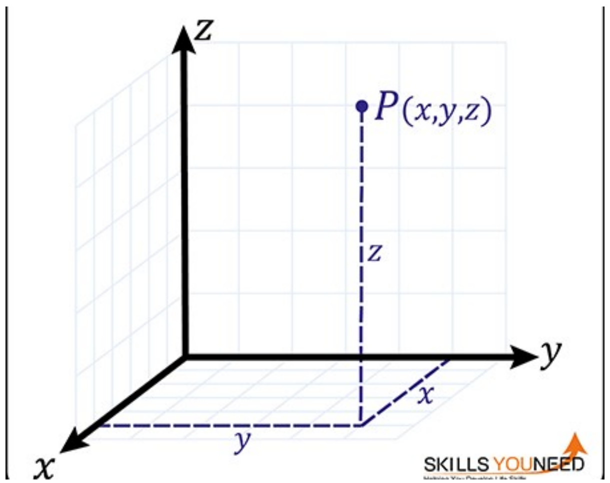
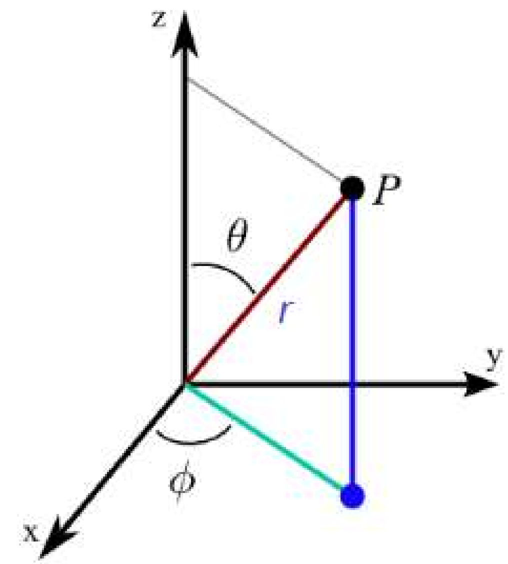
Schrodinger Wave Equation for H atom

$$-\left[\frac{h^2}{8\pi^2 m}\left(\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}+\frac{\partial^2}{\partial z^2}\right)-\frac{e^2}{4\pi\epsilon_0 r}\right]\Psi(x,y,z)=E\Psi(x,y,z)$$



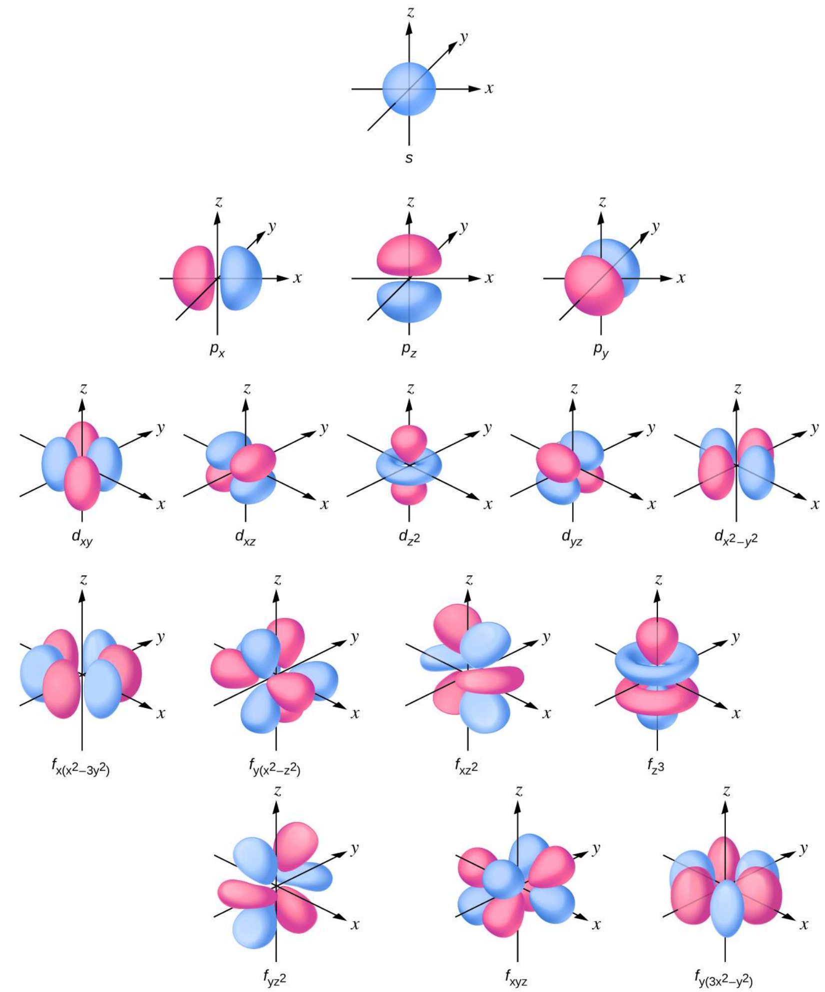
$$\left\{-\frac{\hbar^2}{2\mu r^2}\left[\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right)+\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right)+\frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\varphi^2}\right]-\frac{e^2}{4\pi\epsilon_0 r}\right\}\psi(r,\theta,\varphi)=E\psi(r,\theta,\varphi)$$



$$\psi(r,\theta,\varphi)=R(r)Y(\theta,\varphi)$$

Quantum numbers

n	*l*	*m_l*	m_s	Number of orbitals	Orbital Name	Number of electrons	Total Electrons
1 (K shell)	0	0	½ - ½	1	1*s*	2	2
2 (L Shell)	0	0	½ - ½	1	2*s*	2	8
	1	-1, 0, +1	½ - ½	3	2*p*	6	
3 (M-shell)	0	0	½ - ½	1	3*s*	2	18
	1	-1, 0, +1	½ - ½	3	3*p*	6	
	2	-2, -1, 0, +1, +2	½ - ½	5	3*d*	10	
4 (L-shell)	0	0	½ - ½	1	4*s*	2	32
	1	-1, 0, +1	½ - ½	3	4*p*	6	
	2	-2, -1, 0, +1, +2	½ - ½	5	4*d*	10	
	3	-3, -2, -1, 0, +1, +2, +3	½ - ½	7	4*f*	14	



$$\psi_{n,l,m_l}(r,\theta,\phi) = R_{n,l}(r)\,Y_{l,m_l}(\theta,\phi)$$

Radial and angular wavefunctions

$$\psi_{n,l,m_l}(r,\theta,\phi) = R_{n,l}(r)Y_{l,m_l}(\theta,\phi)$$

$$R_{10}(r) = \frac{2}{\sqrt{a_0^3}}e^{-r/a_0}, \qquad R_{20}(r). = \frac{1}{2\sqrt{2}\sqrt{a_0^3}}\left(2-\frac{r}{a_0}\right)e^{-r/2a_0}$$

$$R_{21}(r) = \frac{1}{2\sqrt{6}\sqrt{a_0^3}}\frac{r}{a_0}e^{-r/2a_0}$$

$$R_{30}(r) = \frac{1}{81\sqrt{3}\sqrt{a_0^3}}\left(27-18\frac{r}{a_0}+2\frac{r^2}{a_0^2}\right)e^{-r/3a_0}$$

$$R_{31}(r) = \frac{4}{81\sqrt{6}\sqrt{a_0^3}}\left(6-\frac{r}{a_0}\right)\frac{r}{a_0}e^{-r/3a_0}, \quad R_{32}(r) = \frac{4}{81\sqrt{30}\sqrt{a_0^3}}\frac{r^2}{a_0^2}e^{-r/3a_0}$$

Angular Wave Function Y_{l,m_l} for $l = 0, 1$

l	m_l	Y_{l,m_l}
0	0	$\frac{1}{2\sqrt{\pi}}$
1	−1	$-\frac{1}{2}\sqrt{\frac{3}{2\pi}}\sin\theta\, e^{-i\phi}$
1	0	$\frac{1}{2}\sqrt{\frac{3}{\pi}}\cos\theta$
1	1	$\frac{1}{2}\sqrt{\frac{3}{2\pi}}\sin\theta\, e^{+i\phi}$

Radial Probability Distribution

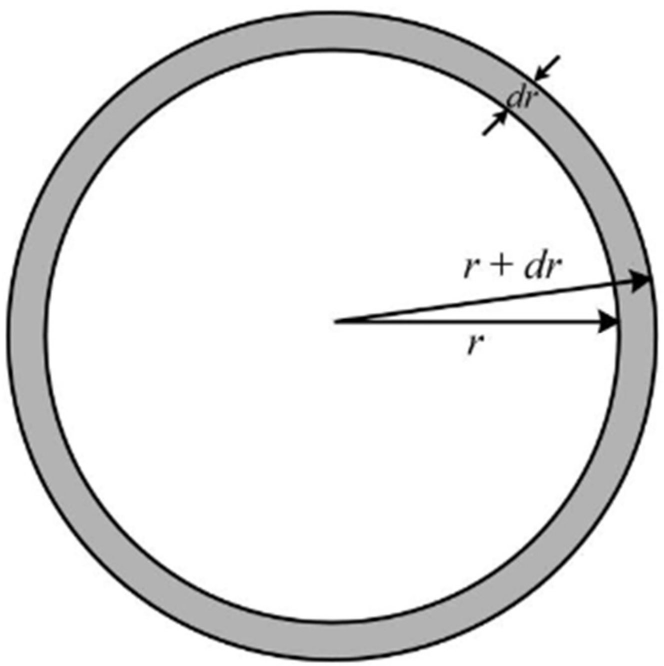
Complex conjugate $\Psi = a + ib$

$\Psi^* = a - ib$

$|\Psi|^2$ *or* $\Psi\Psi^*$ *is proportional to the probability of finding a particle at a given time*

$$P \propto \Psi\Psi^* \mathrm{dxdydz} = \Psi\Psi^* \partial V$$

$$Radial\ probability = R_{n,l}^2 \times dV$$



$$dV = \frac{4}{3}\pi(r+dr)^3 - \frac{4}{3}\pi r^3$$

$$= \frac{4}{3}\pi(r^3 + dr^3 + 3r^2dr + 3r\,dr^2) - \frac{4}{3}\pi r^3$$

$$= \frac{4}{3}\pi r^3 + \frac{4}{3}\pi dr^3 + 4\pi r^2 dr + 4\pi r\,dr^2 - \frac{4}{3}\pi r^3$$

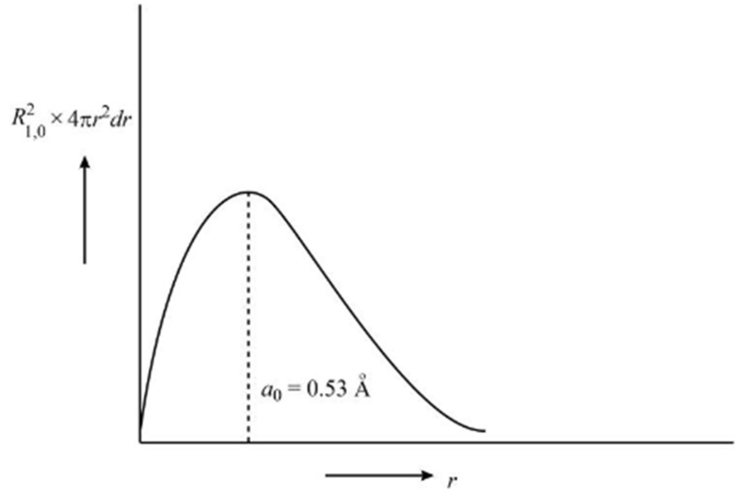
$$dV = \frac{4}{3}\pi dr^3 + 4\pi r^2 dr + 4\pi r\,dr^2$$

since dr^3 and dr^2 are very small terms, these can be supposed to be equal to zero and hence the above equation becomes.

Radial probability of finding the electron within the small radial shell of thickness of dr

$$= R^2_{n,l} \times dv = R^2_{n,l} \times 4\pi r^2 dr$$

Radial Probability Distribution

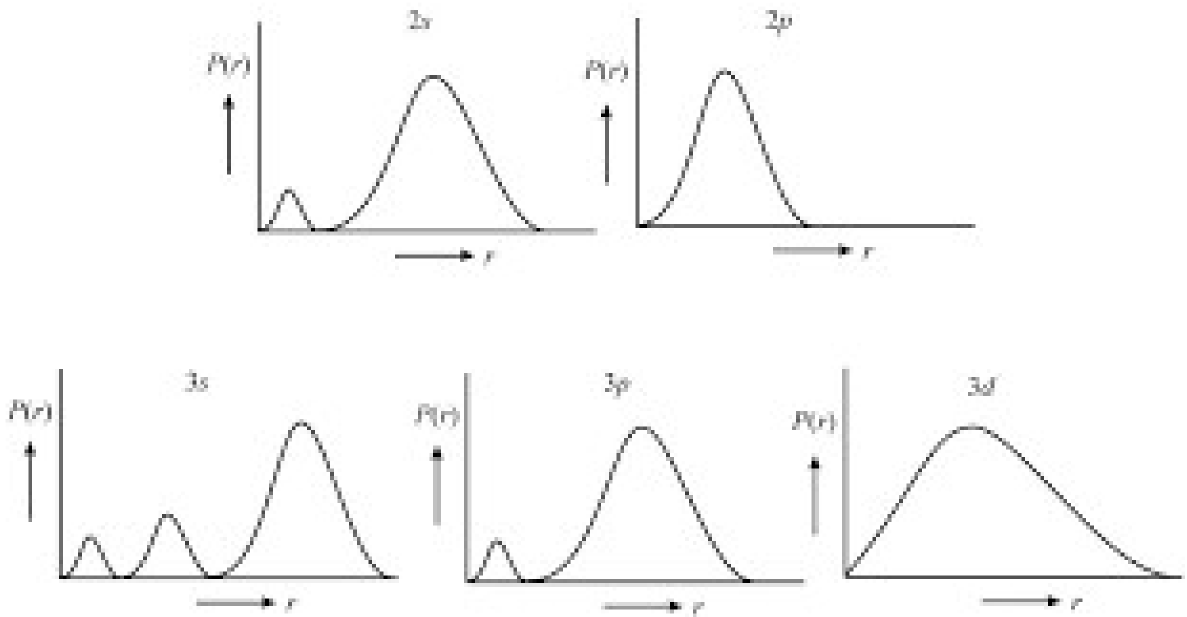


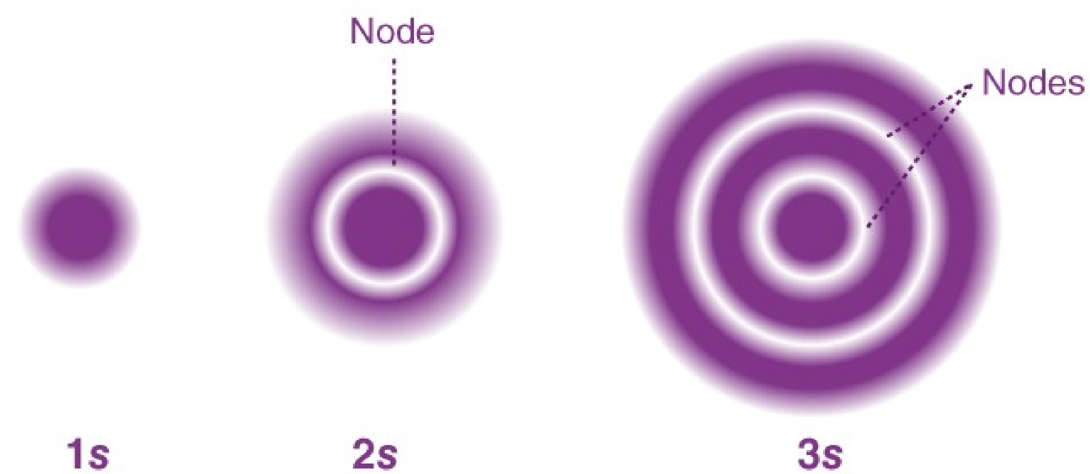
$$R_{10}(r) = \frac{2}{\sqrt{a_0^3}} e^{-r/a_0}, \qquad R_{20}(r). = \frac{1}{2\sqrt{2}\sqrt{a_0^3}} \left(2 - \frac{r}{a_0}\right) e^{-r/2a_0}$$

$$R_{21}(r) = \frac{1}{2\sqrt{6}\sqrt{a_0^3}} \frac{r}{a_0} e^{-r/2a_0}$$

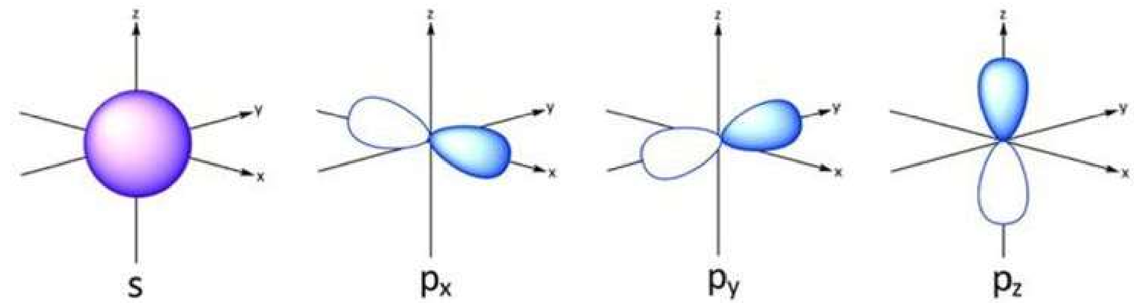
$$R_{30}(r) = \frac{1}{81\sqrt{3}\sqrt{a_0^3}} \left(27 - 18\frac{r}{a_0} + 2\frac{r^2}{a_0^2}\right) e^{-r/3a_0}$$

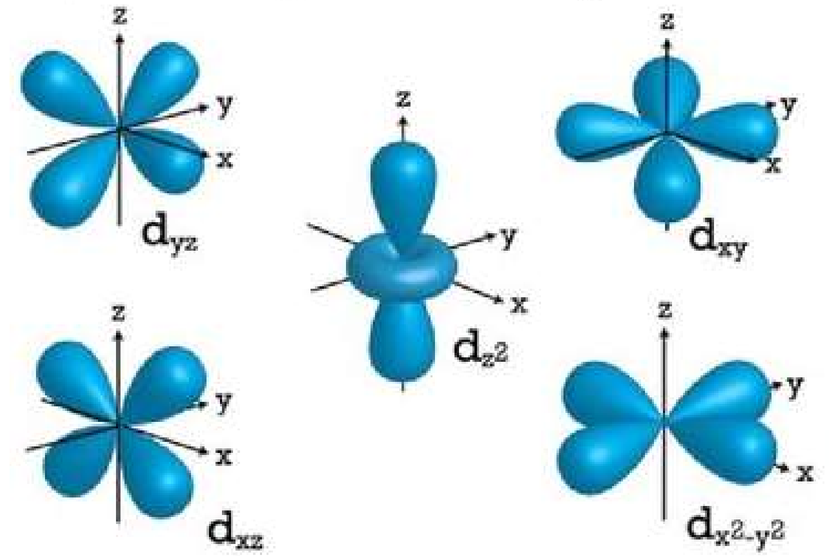
$$R_{31}(r) = \frac{4}{81\sqrt{6}\sqrt{a_0^3}} \left(6 - \frac{r}{a_0}\right) \frac{r}{a_0} e^{-r/3a_0}, \quad R_{32}(r) = \frac{4}{81\sqrt{30}\sqrt{a_0^3}} \frac{r^2}{a_0^2} e^{-r/3a_0}$$

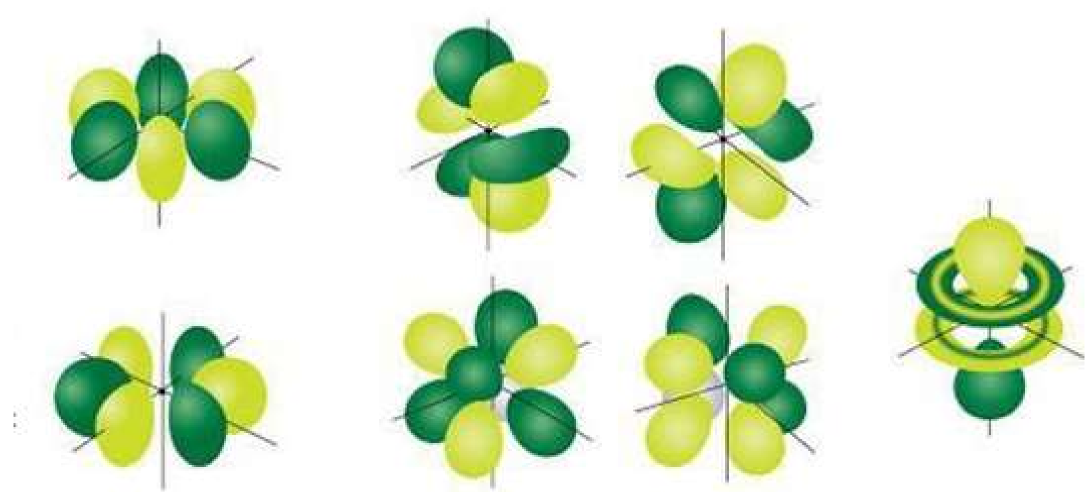


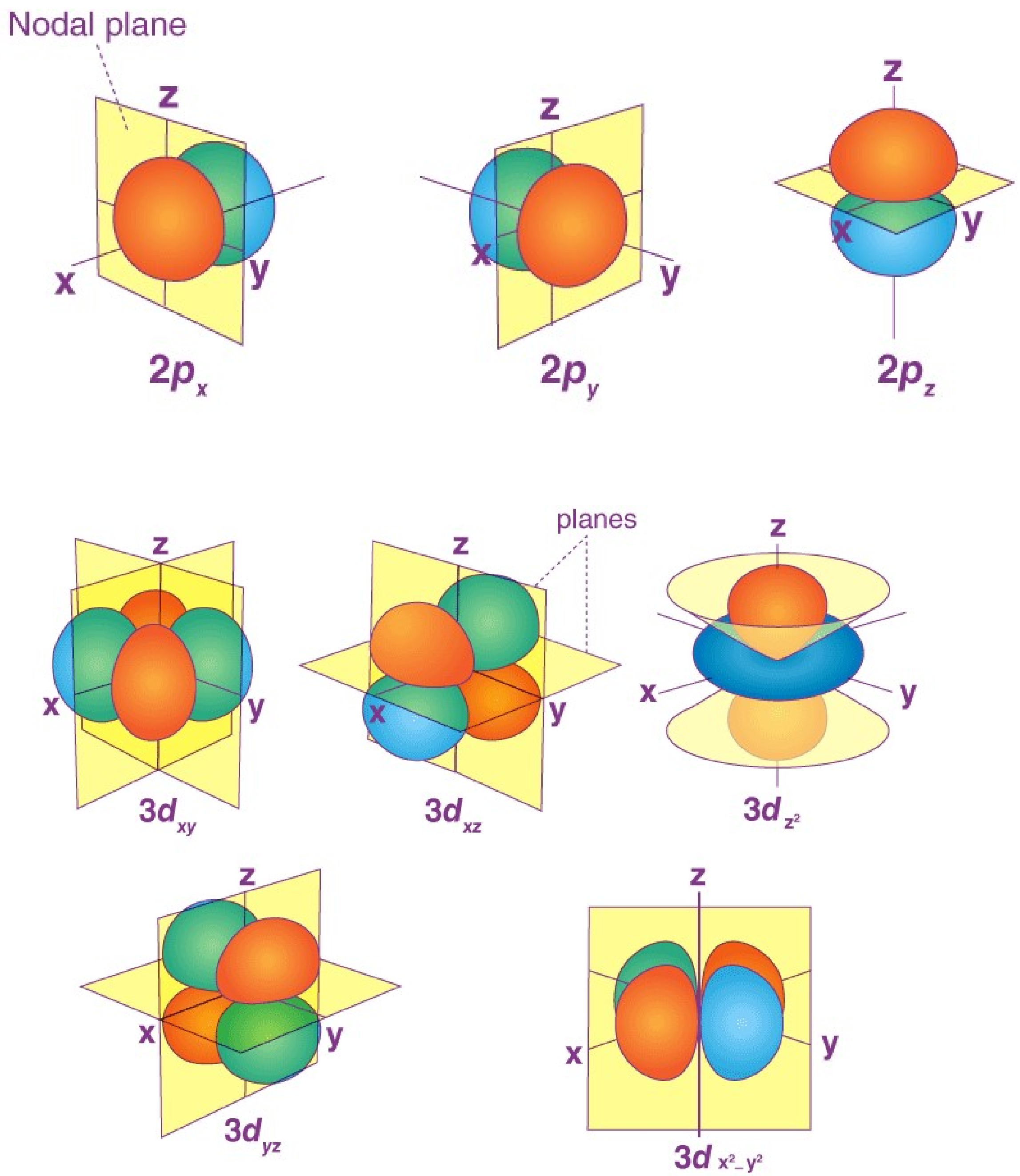


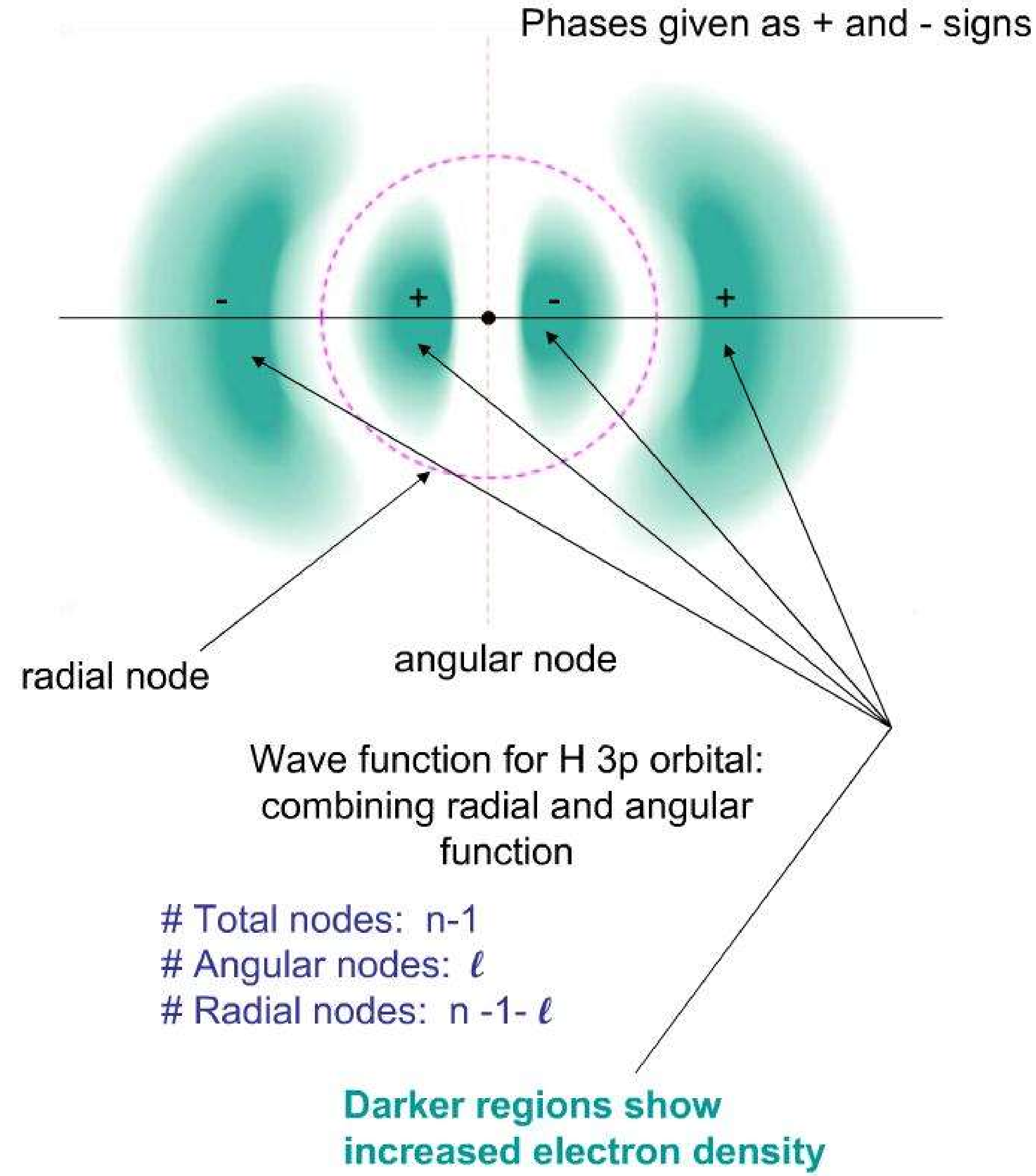
n	ℓ	m_ℓ		$\Psi_{n\ell m_\ell}(r,\theta,\varphi)$
3	0	0	3s	$\frac{1}{81\sqrt{3\pi}a_0^{3/2}}\left[27-18\frac{r}{a_0}+2\frac{r^2}{a_0^2}\right]e^{-r/3a_0}$
3	1	0	3p	$\frac{\sqrt{2}}{81\sqrt{\pi}a_0^{3/2}}\left[6-\frac{r}{a_0}\right]\frac{r}{a_0}e^{-r/3a_0}\cos\theta$
3	1	±1	3p	$\frac{1}{81\sqrt{\pi}a_0^{3/2}}\left[6-\frac{r}{a_0}\right]\frac{r}{a_0}e^{-r/3a_0}\sin\theta e^{+i\phi}$
3	2	0	3d	$\frac{1}{81\sqrt{6\pi}a_0^{3/2}}\frac{r^2}{a_0^2}e^{-r/3a_0}(3\cos^2\theta-1)$
3	2	±1	3d	$\frac{1}{81\sqrt{\pi}a_0^{3/2}}\frac{r^2}{a_0^2}e^{-r/3a_0}\sin\theta\cos\theta e^{+i\phi}$
3	2	±2	3d	$\frac{1}{162\sqrt{\pi}a_0^{3/2}}\frac{r^2}{a_0^2}e^{-r/3a_0}\sin^2\theta e^{+i2\phi}$



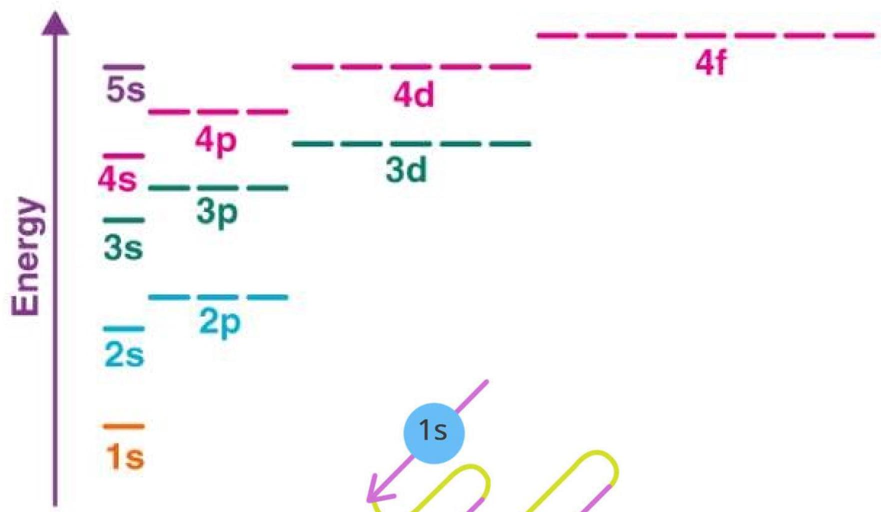


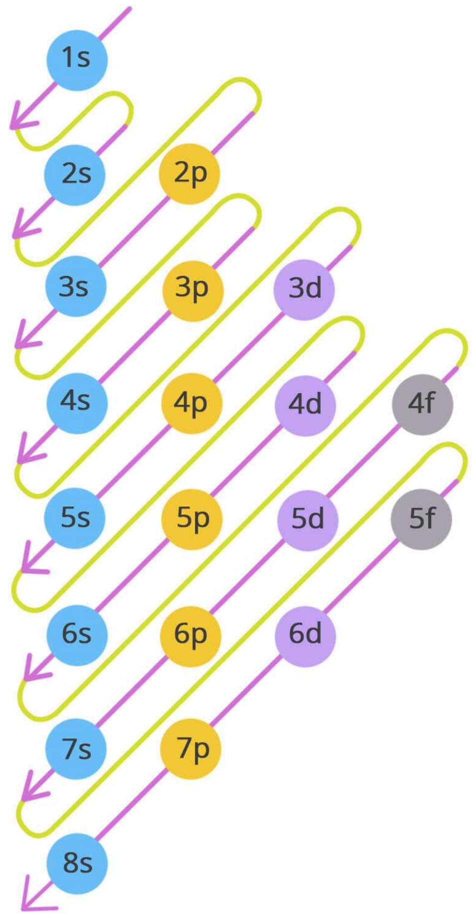



Nodal plane
z
x
y
$2p_x$
$2p_y$
$2p_z$
planes
$3d_{xy}$
$3d_{xz}$
$3d_{z^2}$
$3d_{yz}$
$3d_{x^2-y^2}$


Phases given as + and - signs
-
+
-
+
radial node
angular node
Wave function for H 3p orbital: combining radial and angular function
Total nodes: n-1
Angular nodes: ℓ
Radial nodes: n -1- ℓ
Darker regions show increased electron density

Aufbau's principle



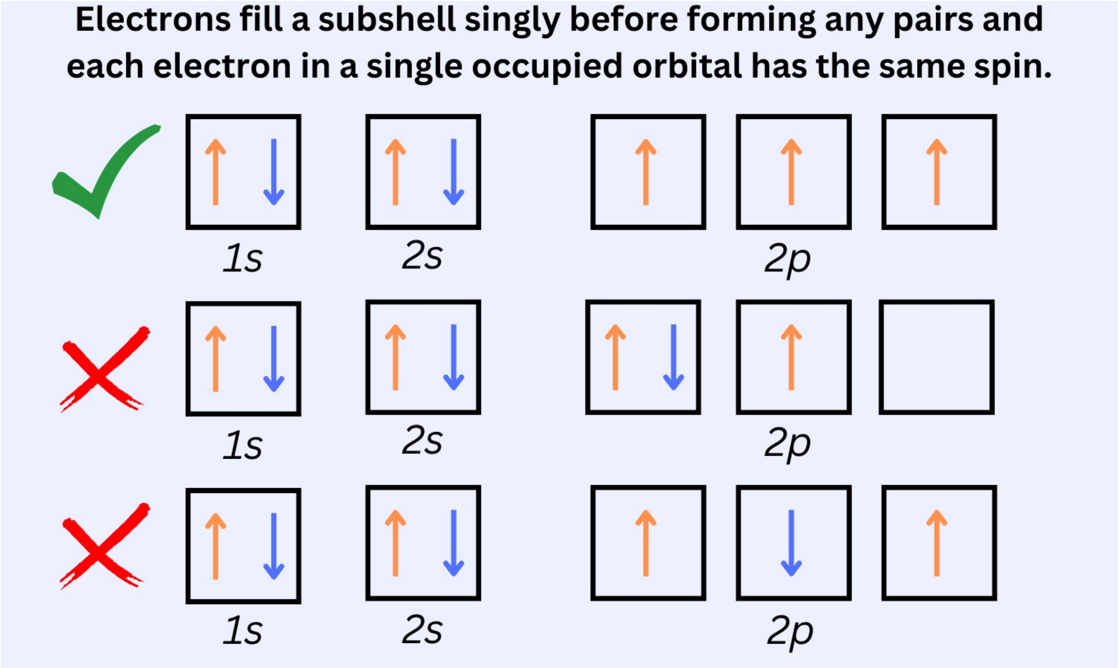


Element	Electron Configuration	Element	Electron Configuration
H	$1s^1$	Na	$1s^2 2s^2 2p^6 3s^1$
He	$1s^2$	Mg	$1s^2 2s^2 2p^6 3s^2$
Li	$1s^2 2s^1$	Al	$1s^2 2s^2 2p^6 3s^2 3p^1$
Be	$1s^2 2s^2$	Si	$1s^2 2s^2 2p^6 3s^2 3p^2$
B	$1s^2 2s^2 2p^1$	P	$1s^2 2s^2 2p^6 3s^2 3p^3$
C	$1s^2 2s^2 2p^2$	S	$1s^2 2s^2 2p^6 3s^2 3p^4$
N	$1s^2 2s^2 2p^3$	Cl	$1s^2 2s^2 2p^6 3s^2 3p^5$
O	$1s^2 2s^2 2p^4$	Ar	$1s^2 2s^2 2p^6 3s^2 3p^6$
F	$1s^2 2s^2 2p^5$	K	$1s^2 2s^2 2p^6 3s^2 3p^6 4s^1$
Ne	$1s^2 2s^2 2p^6$	Ca	$1s^2 2s^2 2p^6 3s^2 3p^6 4s^2$

Hund's Rule

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 (to maximize total spin).



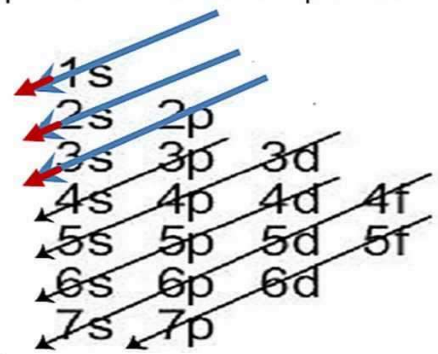
Pauli's exclusion principle

According to the Pauli Exclusion Principle, two electrons within an atom can't possess identical sets of four electronic quantum numbers.

Electron Configuration Chart

s holds up to **2** **p** holds up to **6** **d** holds up to **10**

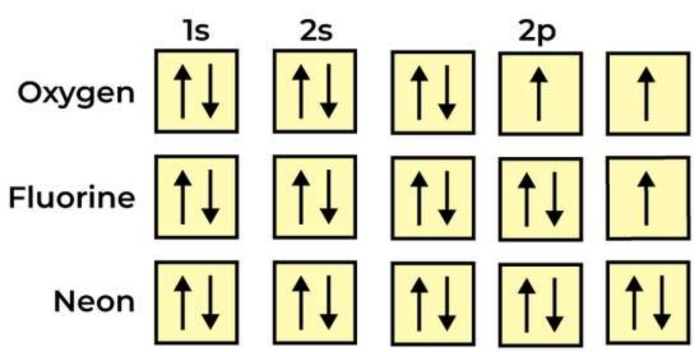
11
Na
Sodium
22.99



$1s^2 2s^2 2p^6 3s^1$

Pauli Exclusion Principle

Examples



Electron	n	l	m	s
1s 1st Electron	1	0	0	1/2
1s 2nd Electron	1	0	0	-1/2
2s 1st Electron	2	0	0	1/2
2s 2nd Electron	2	0	0	-1/2
2p 1st Electron	2	1	-1	1/2
2p 2nd Electron	2	1	0	1/2
2p 3rd Electron	2	1	1	1/2
2p 4th Electron	2	1	-1	-1/2
2p 5th Electron	2	1	0	-1/2
2p 6th Electron	2	1	1	-1/2
3s 1st Electron	3	0	0	1/2