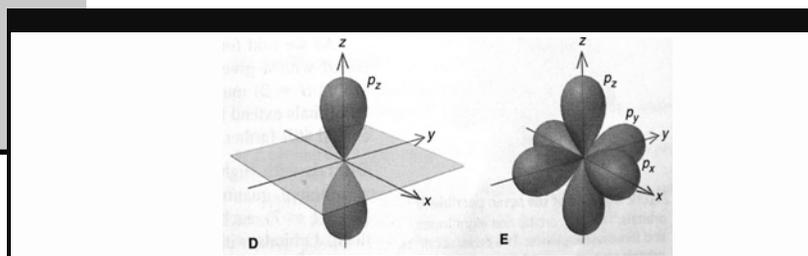


QUANTUM-MECHANICAL MODEL OF THE ATOM

GENERAL CHEMISTRY

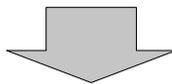
by Dr. Istadi



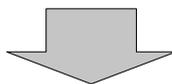
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Quantum Mechanics ?

- Dual nature of matter and energy
- The uncertainty principle
- The wave nature of objects on the atomic scale



Quantum Mechanics



Erwin Schrodinger (1926) ==> equation as the basis for the quantum-mechanical model of the hydrogen atom

The model describes an atom that has certain allowed quantities of energy due to the allowed wavelike behavior of an electron whose exact location is impossible to know

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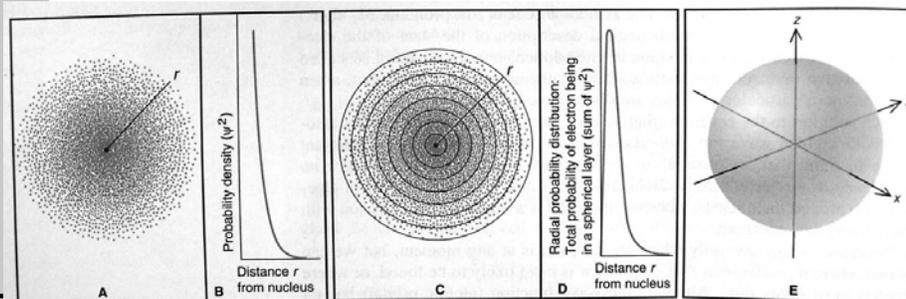
Atomic Orbital & Probable Location of Electron

- The electron's wave function (ψ , atomic orbital) is mathematical description of the electron's wavelike behavior in an atom
- Schrödinger Equation: $\mathbf{H}\psi = \mathbf{E}\psi$
- E : energy of atom; ψ : wave function, H : Hamiltonian operator
- In complete form:

$$\left[-\frac{\hbar^2}{8\pi^2 m_e} \left(\frac{d^2}{dx^2} + \frac{d^2}{dy^2} + \frac{d^2}{dz^2} \right) + V(x, y, z) \right] \psi(x, y, z) = E\psi(x, y, z)$$
- Each wave function is associated with one of the atom's allowed energy states
- Each solution to the equation (each energy state of the atom) is associated with a given wave function ==> **Atomic Orbital**
- In Bohr's model, orbit was an electron's path around the nucleus
- Here, orbital is mathematical function with no direct physical meaning

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Electron Probability Density



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- An electron density diagram and a radial probability distribution plot show how the electron occupies the space near the nucleus for a particular energy level.
- We cannot know precisely where the electron is at any moment, but we can describe where it probably is, that is where it is most likely to be found
- Although the wave function (atomic orbital) has no direct physical meaning, the ψ^2 (probability density) measures the probability that the electron can be found within a particular tiny volume of the atom
- For a given energy level, we can depict this probability with an electron probability density diagram or an **electron density diagram**

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- Electron density diagrams are called **electron clouds**
- **The electron moves around the nucleus that would appear as a “cloud” of electron positions.**
- **The electron cloud is an imaginary picture of the electron changing its position rapidly over time**
- **It does not mean that an electron is a diffuse cloud of charge**
- **The electron probability density decreases with distance from the nucleus along a line r .**

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Quantum Number of an Atomic Orbital

- When the absorbs energy, it exists in an excited state and the region of space occupied by the electron ==> a different atomic orbital (wave function)
- An atomic orbital is specified by **three quantum numbers**:
 - **Principal Quantum Number (n):**
 - positive integer (1,2,3,...)
 - Indicates the **relative size of the orbital** and therefore the distance from the nucleus of the peak in the radial probability plot
 - specifies the energy level of the H atom where *the higher the n value, the higher the energy level.*
 - Example: H atom, when electron ==> $n=1$ ==> ground state ==> has lower energy; when electron ==> $n=2$ ==> excited state ==> has higher energy

■ **Angular momentum quantum number (l):**

- an integer from 0 to $n-1$
- Indicates the shape of the orbital, sometimes called as "*orbital-shape quantum number*"
- n limits l
- Example: for orbital with $n=1$ ==> $l=0$; $n=2$ ==> $l=0,1$
- **Magnetic quantum number (m_l):**
 - an integer from -1 through 0 to +1
 - prescribes the orientation of the orbital in the space around the nucleus, sometimes called as "*orbital-orientation quantum number*"
 - l sets the possible values of m_l .
 - Example: $l=0$ ==> $m_l=0$; $l=1$ ==> $m_l=-1,0,+1$
 - the number of possible m_l values equals the number of orbitals, which is $2l+1$ for a given l value.

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Hierarchy of Quantum Numbers for Atomic Orbitals

Table 7.2 The Hierarchy of Quantum Numbers for Atomic Orbitals

Name, Symbol (Property)	Allowed Values	Quantum Numbers
Principal, n (size, energy)	Positive integer (1, 2, 3, ...)	1 2 3
Angular momentum, l (shape)	0 to $n - 1$	0 0 1 0 1 2
Magnetic, m_l (orientation)	$-l, \dots, 0, \dots, +l$	0 0 -1 0 +1 0 -1 0 +1 -2 -1 0 +1 +2

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- The energy states and orbitals of the atom are described with specific terms and associated with one or more quantum numbers:
 1. **Level:** the atom's energy **levels**, or **shells**, are given by the n value (the smaller the n value, the lower the energy level and the greater the probability of the electron being closer to the nucleus)
 2. **Sublevel:** the atom's levels contain **sublevels**, or **subshells**, which designate the orbital shape:
 - $l=0$ is an **s** sublevel
 - $l=1$ is a **p** sublevel
 - $l=2$ is a **d** sublevel
 - $l=3$ is a **f** sublevel

s: sharp, **p:** principal, **d:** diffuse, **f:** fundamental
 The sublevel with $n=2$ and $l=0$ ==> **2s** sublevel

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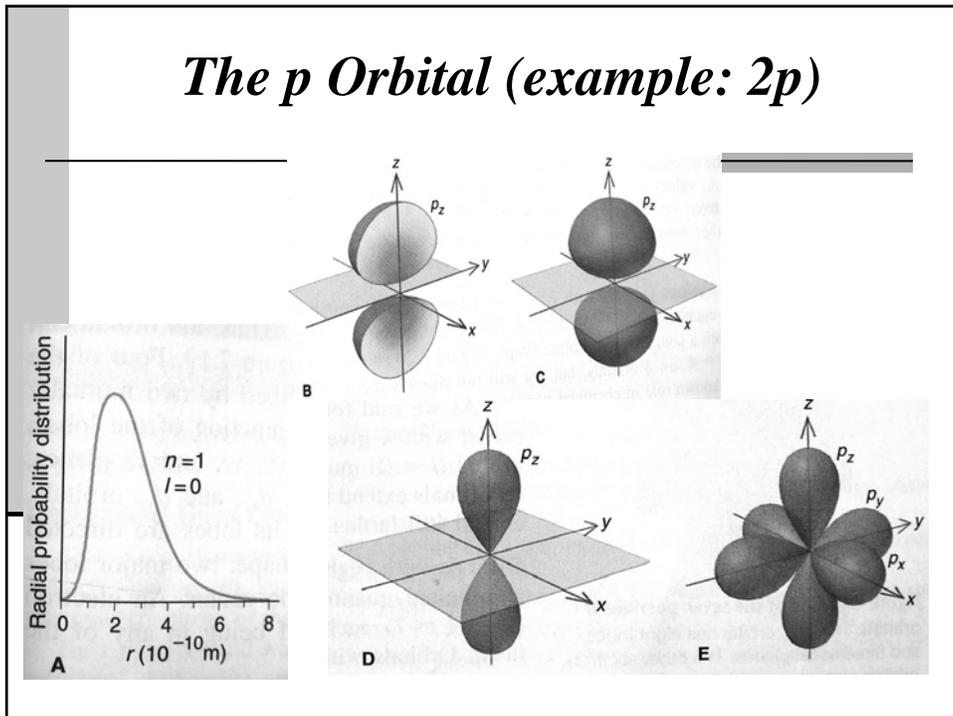
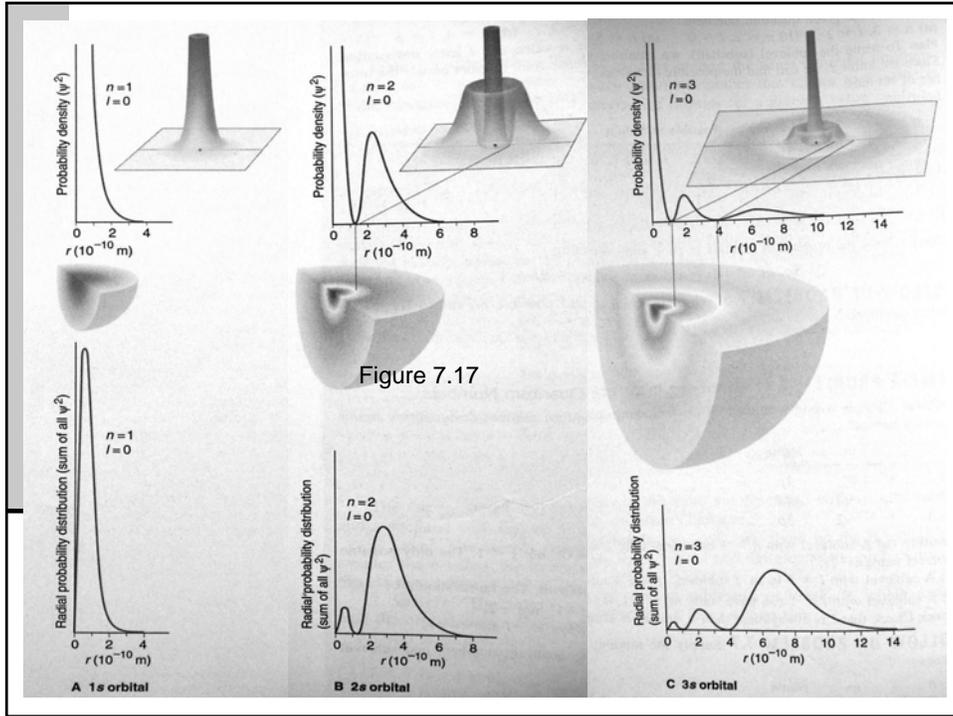
3. **Orbital:** each allowed combination of n , l , and m_l values specifies one of the atom's orbitals.
- Thus the three quantum numbers describes an orbital expressing its size (energy), shape, and spatial orientation.
 - Example: from the hierarchy $\implies n=2, l=0$, and $m_l=0$.
 - Example: **3p** sublevel has three orbitals:
 - one with $n=3, l=1$, and $m_l=-1$
 - another with $n=3, l=1$ and $m_l=0$
 - and third with $n=3, l=1$, and $m_l=+1$
- Give the name, magnetic quantum number, and number of orbital for the following quantum numbers:
- $n=3, l=2$
 - $n=2, l=0$
 - $n=5, l=1$

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Shapes of Atomic Orbitals: *s Orbital*

- The **s** orbital:
 - $l=0 \rightarrow$ spherical shape with nucleus at the center \rightarrow s orbital
 - for H atom's ground state \rightarrow the electron probability density is highest at the nucleus (Fig. 7.17A)
 - Fig. 7.17B \rightarrow Because the 2s orbital is larger than the 1s, an electron in 2s spend more time farther from the nucleus than when it occupies the 1s.
 - Fig. 7.17C \rightarrow the highest radial probability is at the greatest distance from the nucleus
 - An s orbital has a spherical shape, so it can have only one orientation and, thus only one value for the magnetic quantum number: for any s orbital, $m_l=0$

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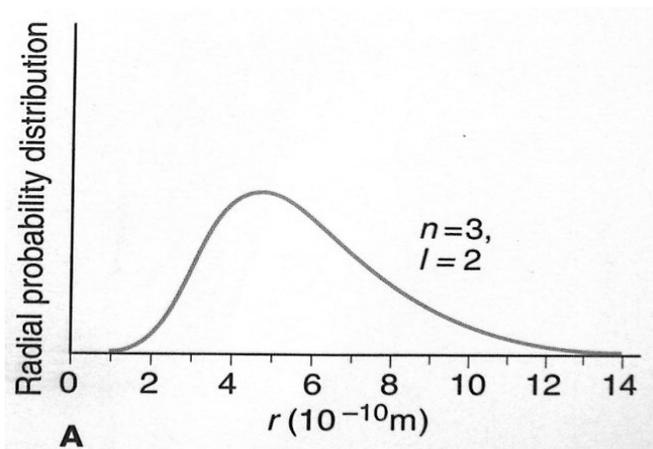


- An orbital with $l=1$ has two regions (*lobes*) of high probability, one on either side of the nucleus, and is called a p orbital.
- In the previous figure, the nucleus lies at the nodal plane of the dumbbell-shaped orbital.
- The maximum value of l is $n-1 \implies$ only levels with $n=2$ or higher can have a p orbital.
- Therefore, the lowest energy p orbital is the $2p$.
- Unlike an s orbital, each p orbital does have a specific orientation in space. The $l=1 \implies m_l = -1, 0, +1 \implies$ three mutually perpendicular p orbitals. They are identical in size, shape and energy, but differing only in orientation
- p orbital associates to x , y , and z axes $\implies p_x, p_y$, and p_z

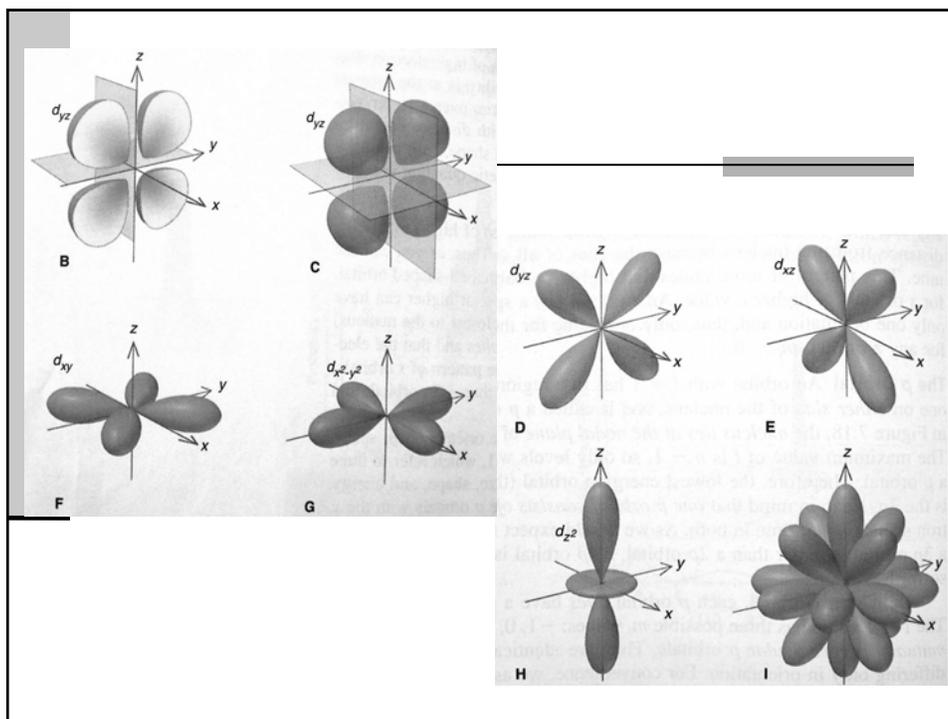
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The d Orbital (example: 3d)

- Radial probability distribution plot



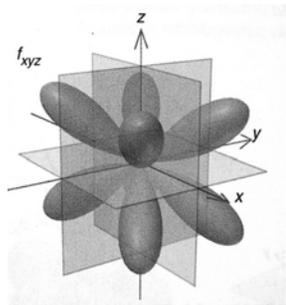
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- An orbital with $l=2$ is called a **d** orbital, with 5 possible m_l values (-2, -1, 0, +1, +2).
- **d** orbital can have any one of five different orientations, as depicted in previous figure
- The following is one of the seven possible 4*f* orbitals:

Orbitals with Higher l Values

- Orbitals with $l=3$ are f orbitals and must have a principal quantum number at least $n=4$.
- There are seven f orbitals ($2l + 1 = 7$), each with a complex, multilobed shape
- Orbitals with $l=4$ are g orbitals, but they will not be discussed, because they play no known role in chemical bonding



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Energy Levels of the Hydrogen Atom

- *The energy state of the H atom depends on the principal quantum number n only.*
- An electron in an orbital with a higher n value spends its time farther from the nucleus, so it is higher in energy
- Thus, in the case of H atom only, all four $n=2$ sublevels (one $2s$ and three $2p$) have the same energy.
- and all nine $n=3$ sublevels (one $3s$, three $3p$, and five $3d$) have the same energy

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