Chapter 7
Atomic Structure -2
Quantum Numbers

Dr. Sapna Gupta

Quantum Numbers

According to quantum mechanics, each electron is described by four quantum numbers:

1. Principal quantum number (n)
2. Angular momentum quantum number (l)
3. Magnetic quantum number (m_l)
4. Electron spin quantum number (m_s)

The first three define the wave function for a particular electron. The fourth quantum number refers to the magnetic property of electrons.

A wave function for an electron in an atom is called an atomic orbital (described by three quantum numbers—n, l, m_l).

It describes a region of space with a definite shape where there is a high probability of finding the electron.

- ***Principal quantum number* (*n*)** - designates size of the orbital
- **Integer values**: 1,2,3, and so forth
- The larger the "*n*" value, the greater the average distance from the nucleus
- Correspond to quantum numbers in Bohr's model

- ***Angular momentum quantum number* (*l*)** – shape of the atomic orbital
- **Integer values**: 0 to $n-1$
- 0 = *s* sublevel; 1 = *p* 2 = *d* 3 = *f*

- ***Magnetic quantum number* (m_l)** – orientation of the orbital in space (think in terms of *x*, *y* and *z* axes)
- **Integer values**: $-l$ to 0 to $+l$
- There are 2e- in each orientation

- ***Electron spin quantum number* (m_s)** – describes the spin of an electron that occupies a particular orbital
- **Values**: +1/2 or –1/2
- Electrons will spin opposite each other in the same orbital

TABLE 6.2 Allowed Values of the Quantum Numbers n, ℓ, and m_ℓ

When n is	ℓ can be	When ℓ is	m_ℓ can be
1	only 0	0	only 0
2	0 or 1	0 1	only 0 −1, 0, or +1
3	0, 1, or 2	0 1 2	only 0 −1, 0, or +1 −2, −1, 0, +1, or +2
4	0, 1, 2, or 3	0 1 2 3	only 0 −1, 0, or +1 −2, −1, 0, +1, or +2 −3, −2, −1, 0, +1, +2, or +3

•**When n = 1, l has only one value, 0.**

•When l = 0, m_l has only one value, 0.

So the first shell (n = 1) has one subshell, an *s*-subshell, 1*s.* That subshell, in turn, has one orbital; 2e$^-$.

•**When n = 2, l has two values, 0 and 1.**

•When l = 0, m_l has only one value, 0. So there is a 2*s* subshell with one orbital; 2e$^-$.

•When l = 1, m_l has only three values, -1, 0, 1. So there is a 2*p* subshell with three orbitals; 6e$^-$.

•**When n = 3, l has three values, 0, 1, and 2.**

•When l = 0, m_l has only one value, 0. So there is a 3*s* subshell with one orbital; 2e$^-$.

•When l = 1, m_l has only three values, -1, 0, 1. So there is a 3*p* subshell with three orbitals, 6e$^-$.

•When l = 2, m_l has only five values, -2, -1, 0, 1, 2. So there is a 3*d* subshell with five orbitals; 10e$^-$.

Atomic View of Quantum Numbers

1

n = 1
l = n-1= 0 (s)
m_l = 0
e- = 2

2

n = 2
l = n-1= 0, 1 (s,p)
m_l = 0
-1,0,+1
e- = 2+6

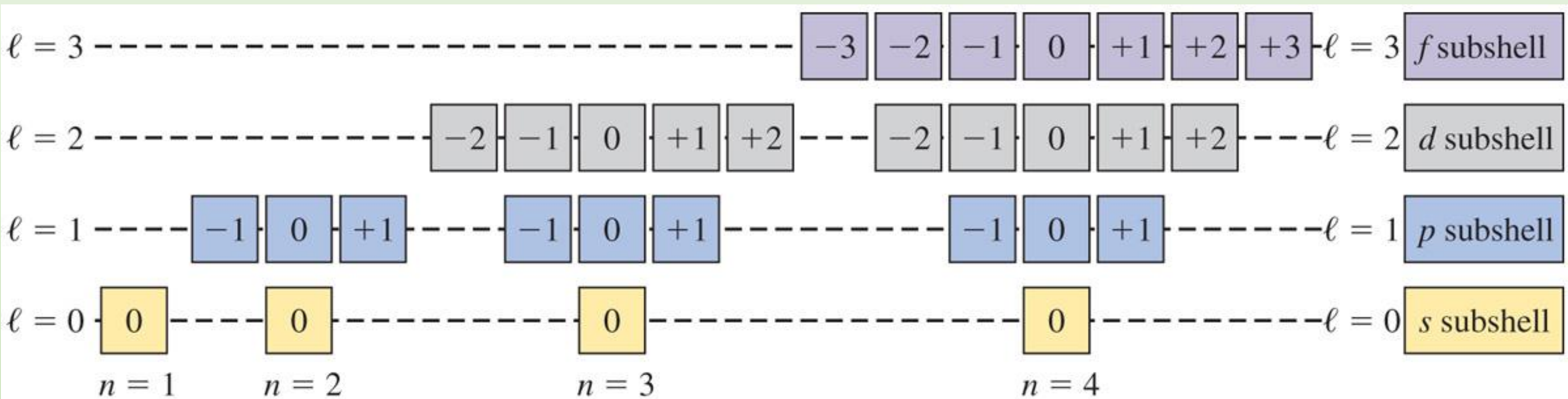
3

n = 3
l = n-1= 0, 1, 2 (s,p,d)
m_l = 0
-1,0,+1
-2,-1,0,+1,+2
e- = 2+6+10

4

n = 4
l = n-1= 0, 1, 2,3 (s,p,d,f)
m_l = 0
-1,0,+1
-2,-1,0,+1,+2
-3,-2,-1,0,+1,+2,+3
e- = 2+6+10+14

Quantum Numbers – another figure



Solved Problem:
Which of the following are permissible sets of quantum numbers?

$n = 4, l = 4, m_l = 0, m_s = ½$
$n = 3, l = 2, m_l = 1, m_s = -½$
$n = 2, l = 0, m_l = 0, m_s = {}^{3}/_{2}$
$n = 5, l = 3, m_l = -3, m_s = ½$

(a) Not permitted. When $n = 4$, the maximum value of l is 3.

(b) Permitted.

(c) Not permitted; m_s can only be +½ or –½.

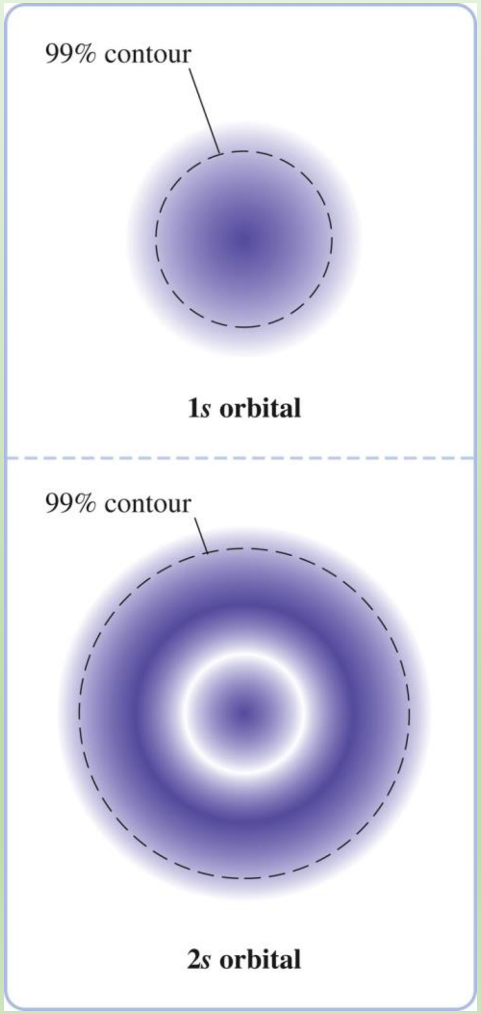
(b) Permitted.

Shapes of Atomic Orbitals

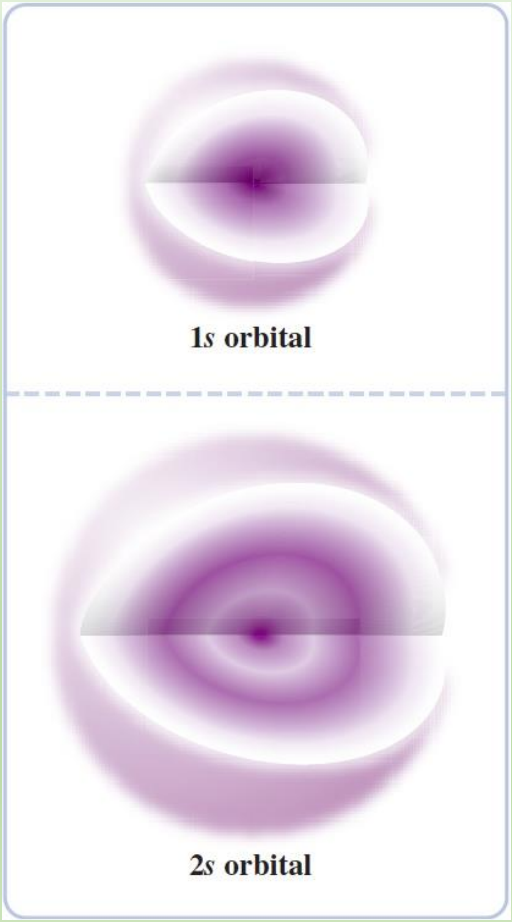
- An *s* orbital is spherical.
- A *p* orbital has two lobes along a straight line through the nucleus, with one lobe on either side.
- A *d* orbital has a more complicated shape.

s - orbital

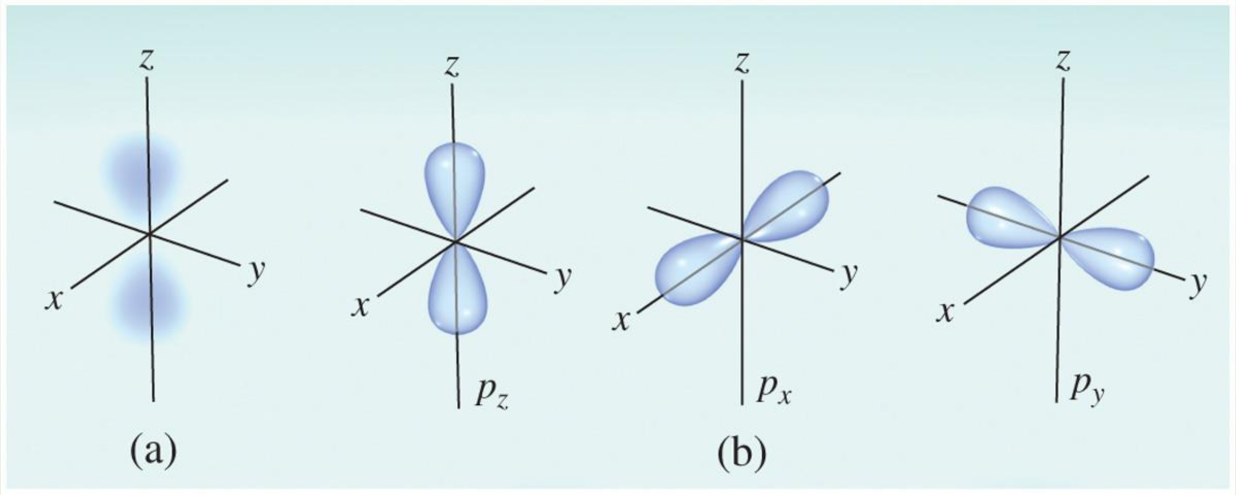
The blue cross-sectional view of a 1*s* orbital and a 2*s* orbital highlights the difference in the two orbitals' sizes.

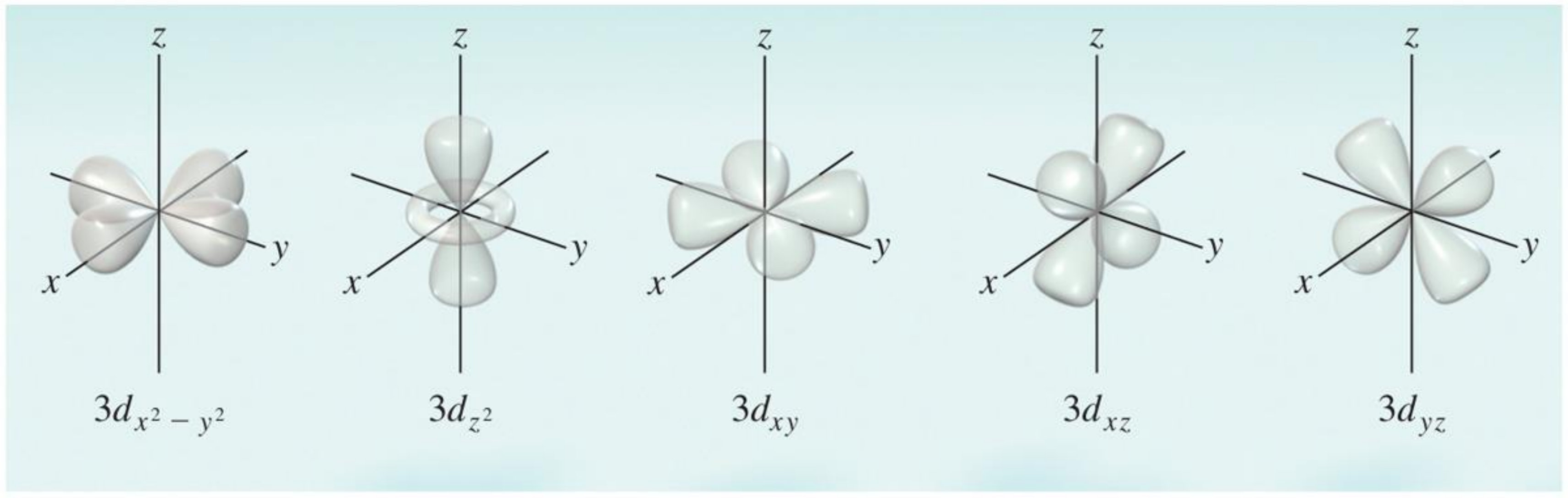


The purple color cutaway diagrams of the 1*s* and 2*s* orbitals give a better sense of them in three dimensions.

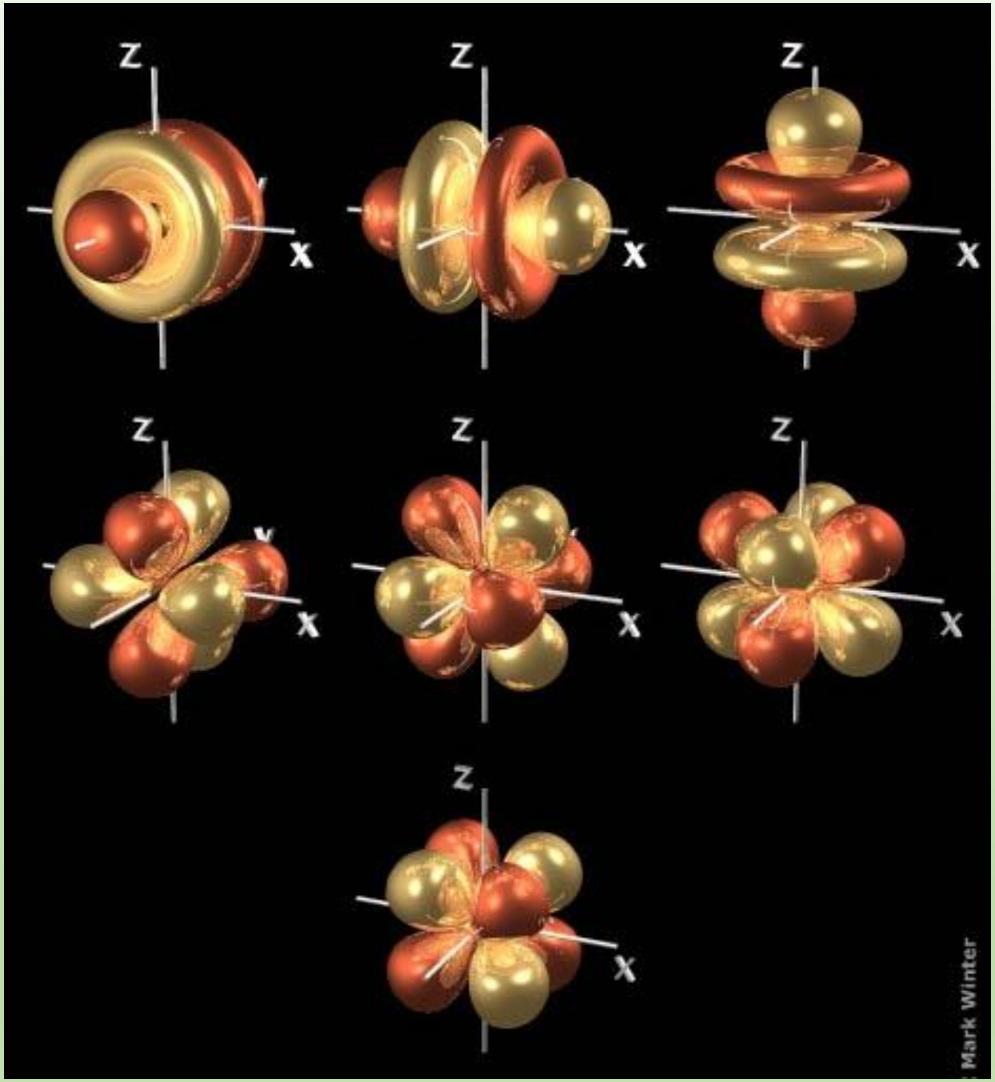


p and d orbitals





F-orbitals



[***Reference***]

All orbitals

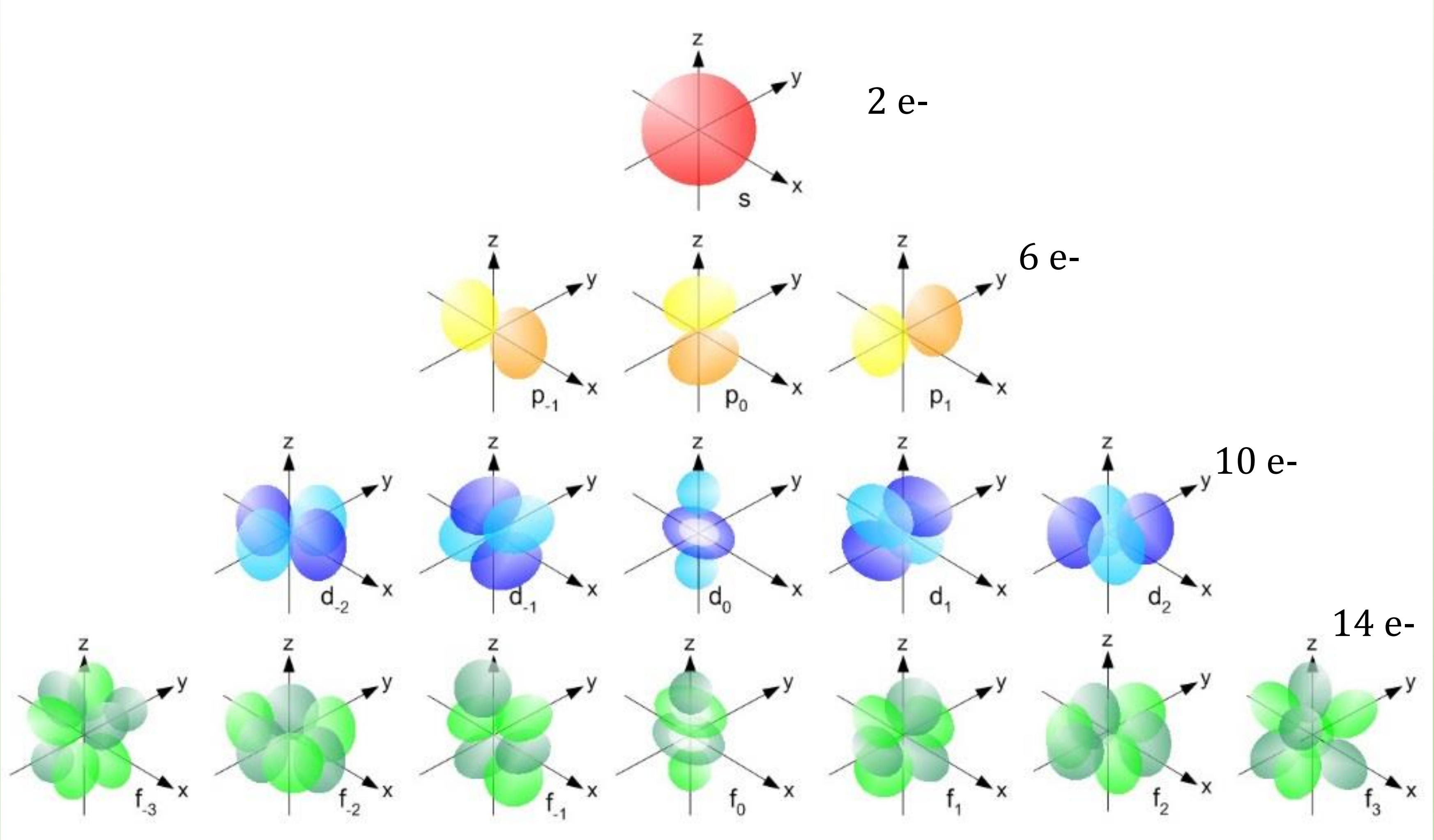


Photo from UC - Davis

Key Points

- Quantum numbers (n, l, m_l, m_s) predict values and possible sets
- Shapes of orbitals