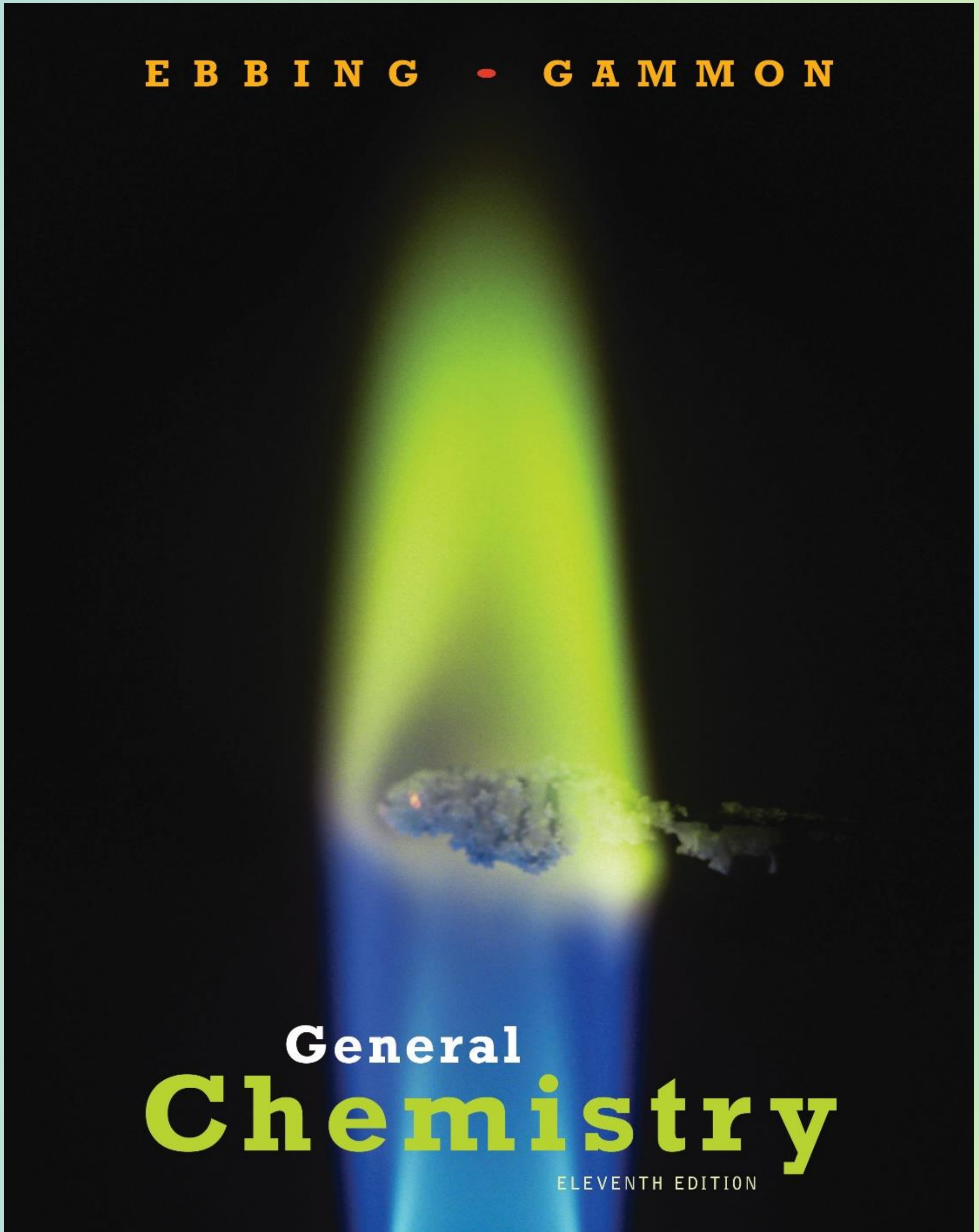


7.5 Quantum Numbers and Atomic Orbitals

- Define *atomic orbital.*
- Define each of the quantum numbers for an atomic orbital.
- State the rules for the allowed values for each quantum number.
- Apply the rules for quantum numbers. Example 7.6
- Describe the shapes of *s*, *p*, and *d* orbitals.

atomic orbital
principal quantum number (n)
angular momentum quantum number (l)
magnetic quantum number (m_l)
spin quantum number (m_s)

Quantum Theory of The Atom

اللهم صلّ وسلّم على نبينا محمد وعلى آله وصحبه أجمعين

- **Note: This is a summary of the lecture. Much more was discussed during the lecture!**
- **Quantum Numbers:**

✓ The allowed values and general meaning of each of the four quantum numbers of an electron in an atom are as follows:

1. Principal Quantum Number (n) Positive value / integer

This quantum number is the one on which the energy of an electron in an atom principally depends.

it can have any positive value: 1, 2, 3, and so on

Letter	K	L	M	N . . .
n	1 <	2 <	3 <	4 . . . Energy

more stable

2. Angular Momentum Quantum Number (l) (Also Called Azimuthal Quantum Number)

This quantum number distinguishes orbitals of given n having different shapes. it can have any integer value from 0 to n − 1.

Letter	s	p	d	f	g . . .
l	0	1	2	3	4 . . .

Energy S < P < d (n=3)

✓ Orbitals of the same *n* but different *l* are said to belong to different *subshells* of a given shell

3. Magnetic Quantum Number (m_l)

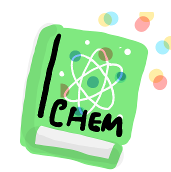
This quantum number distinguishes orbitals of given n and l, that is, of given energy and shape but having a different orientation in space; the allowed values are the integers from −l to +l.

✓ There are 2*l* + 1 orbitals in each subshell of quantum number *l*.

4. Spin Quantum Number (m_s)

This quantum number refers to the two possible orientations of the spin axis of an electron; possible values are +1/2 and -1/2

(Q) State whether each of the following sets of quantum numbers is permissible for an electron in an atom. If a set is not permissible, explain why. Example 7.6



a. $n = 1, l = 1, m_l = 0, m_s = +\frac{1}{2}$	b. $n = 3, l = 1, m_l = -2, m_s = -\frac{1}{2}$
c. $n = 2, l = 1, m_l = 0, m_s = +\frac{1}{2}$	d. $n = 2, l = 0, m_l = 0, m_s = 1$

Table 7.1 Permissible Values of Quantum Numbers for Atomic Orbitals

n	l	m_l*	Subshell Notation	Number of Orbitals in the Subshell
1	0	(0) 1 Orbital	1s	1
2	0	0	2s	1
2	1	(−1, 0, +1) 3 Orbital	2p	3
3	0	0	3s	1
3	1	−1, 0, +1	3p	3
3	2	(−2, −1, 0, +1, +2) 5 Orbital	3d	5
4	0	0	4s	1
4	1	−1, 0, +1	4p	3
4	2	−2, −1, 0, +1, +2	4d	5
4	3	(−3, −2, −1, 0, +1, +2, +3) 7 Orbital	4f	7

Exercise 7.7 Explain why each of the following sets of quantum numbers is not permissible for an orbital.

a. $n = 0, l = 1, m_l = 0, m_s = +\frac{1}{2}$
b. $n = 2, l = 3, m_l = 0, m_s = -\frac{1}{2}$
c. $n = 3, l = 2, m_l = +3, m_s = +\frac{1}{2}$
d. $n = 3, 1 = 2, m_l = +2, m_s = 0$

7.7 a The value of n must be a positive whole number greater than zero. b The values of l range from 0 to $n - 1$. Here, l has a value greater than n. c The values for m_l range from $-l$ to $+l$. Here, m_l has a value greater than that of l. d The values for m_s are $+\frac{1}{2}$ or $-\frac{1}{2}$, not 0.

Example 7.6 Applying the Rules for Quantum Numbers

Gaining Mastery Toolbox

Critical Concept 7.6

An electron in an atom is described by four quantum numbers: the principal quantum number (n), the angular momentum quantum number (l), the magnetic quantum number (m_l), and the spin quantum number (m_s). You need to know the allowed *values* of each quantum number.

Solution Essentials:

Allowed values of the quantum numbers of an atom: n, l, m_l, and m_s

State whether each of the following sets of quantum numbers is permissible for an electron in an atom. If a set is not permissible, explain why.

a. $n = 1, l = 1, m_l = 0, m_s = +\frac{1}{2}$

b. $n = 3, l = 1, m_l = -2, m_s = -\frac{1}{2}$

c. $n = 2, l = 1, m_l = 0, m_s = +\frac{1}{2}$

d. $n = 2, l = 0, m_l = 0, m_s = 1$

Problem Strategy Apply the rules for quantum numbers in order, first to n, then to l and m_l, and finally to m_s. A set of quantum numbers is impermissible if it disobeys any rule.

Solution

a. **Not permissible.** The l quantum number is equal to n; it must be less than n.

b. **Not permissible.** The magnitude of the m_l quantum number (that is, the m_l value, ignoring its sign) must not be greater than l.

c. **Permissible.**

d. **Not permissible.** The m_s quantum number can be only $+\frac{1}{2}$ or $-\frac{1}{2}$.

Answer Check Check that n is a positive integer (it cannot be zero). Also, check that l is a positive integer (but zero is allowed) and that m_l is an integer whose magnitude (its value except for sign) is equal to or less than l. The m_s quantum number can be only $+\frac{1}{2}$ or $-\frac{1}{2}$.

Exercise 7.7 Explain why each of the following sets of quantum numbers is not permissible for an orbital.

a. $n = 0, l = 1, m_l = 0, m_s = +\frac{1}{2}$

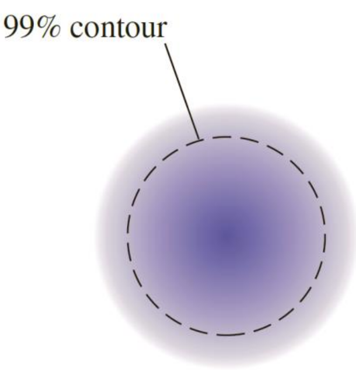
b. $n = 2, l = 3, m_l = 0, m_s = -\frac{1}{2}$

c. $n = 3, l = 2, m_l = +3, m_s = +\frac{1}{2}$

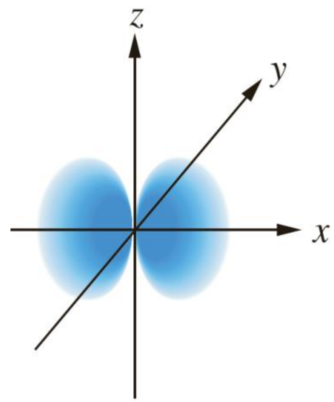
d. $n = 3, 1 = 2, m_l = +2, m_s = 0$

See Problems 7.69 and 7.70.

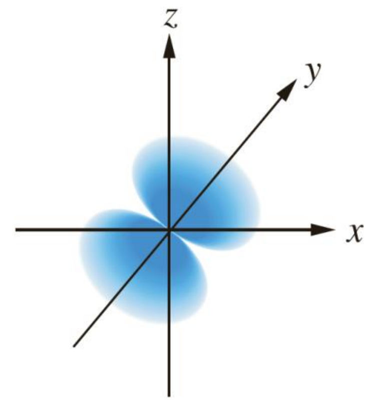
Atomic Orbital Shapes



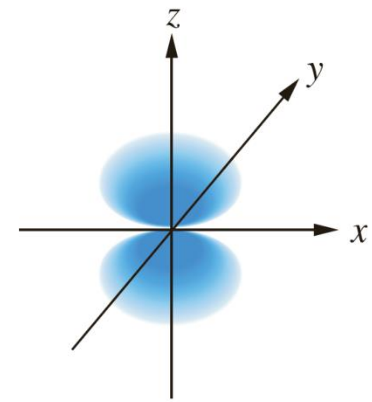
1*s* orbital



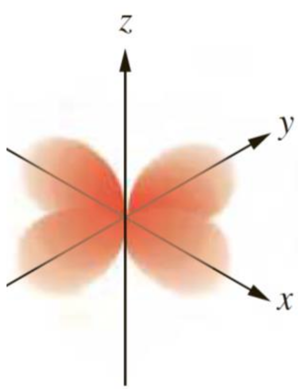
$2p_x$ orbital



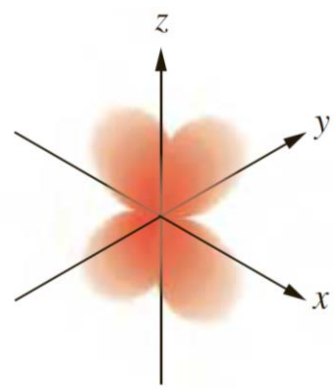
$2p_y$ orbital



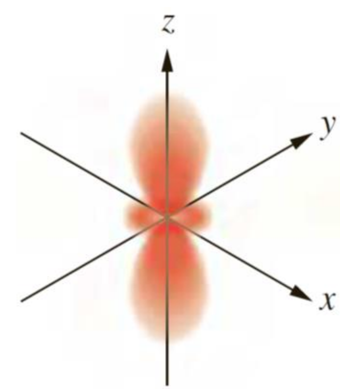
$2p_z$ orbital



$d_{x^2-y^2}$

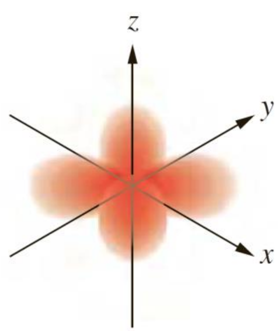


d_{xz}

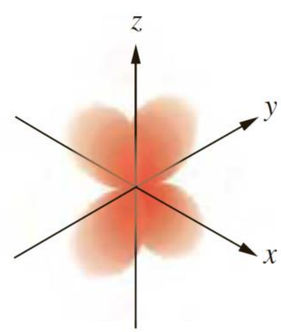


d_{z^2}

Every orbital have a maximum Number Of electrons = 2e-



d_{xy}



d_{yz}

Quantum Numbers

Done by Mas Nafouk

• Principle Quantum No. n

→ refers to Energy & Size

→ Allowed values +ive values [1, 2, ...]

1 2 3 4 ...
K L M N ...

$n \neq 0$
$n \neq -1$

→ $n \propto E \propto$ size of orbitals

• Energy of e^-

- $1e^-$: only depends on n — H, He^+, Li^{+2}
- more than $1e^-$: depends on n and ℓ; $\ell \propto E$ — Fe

→ same n = same Shell.

• Angular momentum Q.No ℓ "Azimuthal"

→ refers to Shape of the Orbitals

→ Allowed values $[0, n-1]$

0 1 2 3 ...
s p d f ..

"spectroscopic terminology" → sharp, principle, diffuse, fundamental

→ Same n = different ℓ = different subshell

→ s, p, d, f has distinctive shapes

→ Shell with Q.No n has n different Kinds of orbitals

• Magnetic Q.No m_ℓ

→ refers to Orientation

→ Allowed values $[+\ell, -\ell]$

→ each ℓ "subshell" has $2\ell+1$ orbitals

→ Ex: $p = +1, 0, -2$ → 3 orbitals

- same E
- same Shape
- different orientation.

• Spin Q. No ms

→ refers to Orientation of the Spin axis of an e^-

→ Allowed Values $+1/2$, $-1/2$

$(1, 2 \ldots)$ $n = 1, 2, 3, 4 \ldots$

$(0, n-1)$ $l = [0], [0, 1], [0, 1, 2], [0, 1, 2, 3]$

Letter Symbols. $= [s], [s, p], [s, p, d], [s, p, d, f]$

$(+l, -l)$ $m_l = [0], [-1, 0, 1], [-2, -1, 0, 1, 2], [-3, -2, -1, 0, 1, 2, 3]$

$l = 0$; $l = 1$; $l = 2$; $l = 3$

$m_s = +\frac{1}{2}$ ↑↓ , $-\frac{1}{2}$ ↑↓

- **For Example** : $4p^3$

- $n = 4$
- $l = 0, 1, 2, 3 = 1$
  (s, p, d, f)
- $m_l = -1, 0, 1$ → [↑] [↑] [↑] → 3 orbitals.
- $m_s = +\frac{1}{2}$

$4p^3$

Done by: Joud Jaber