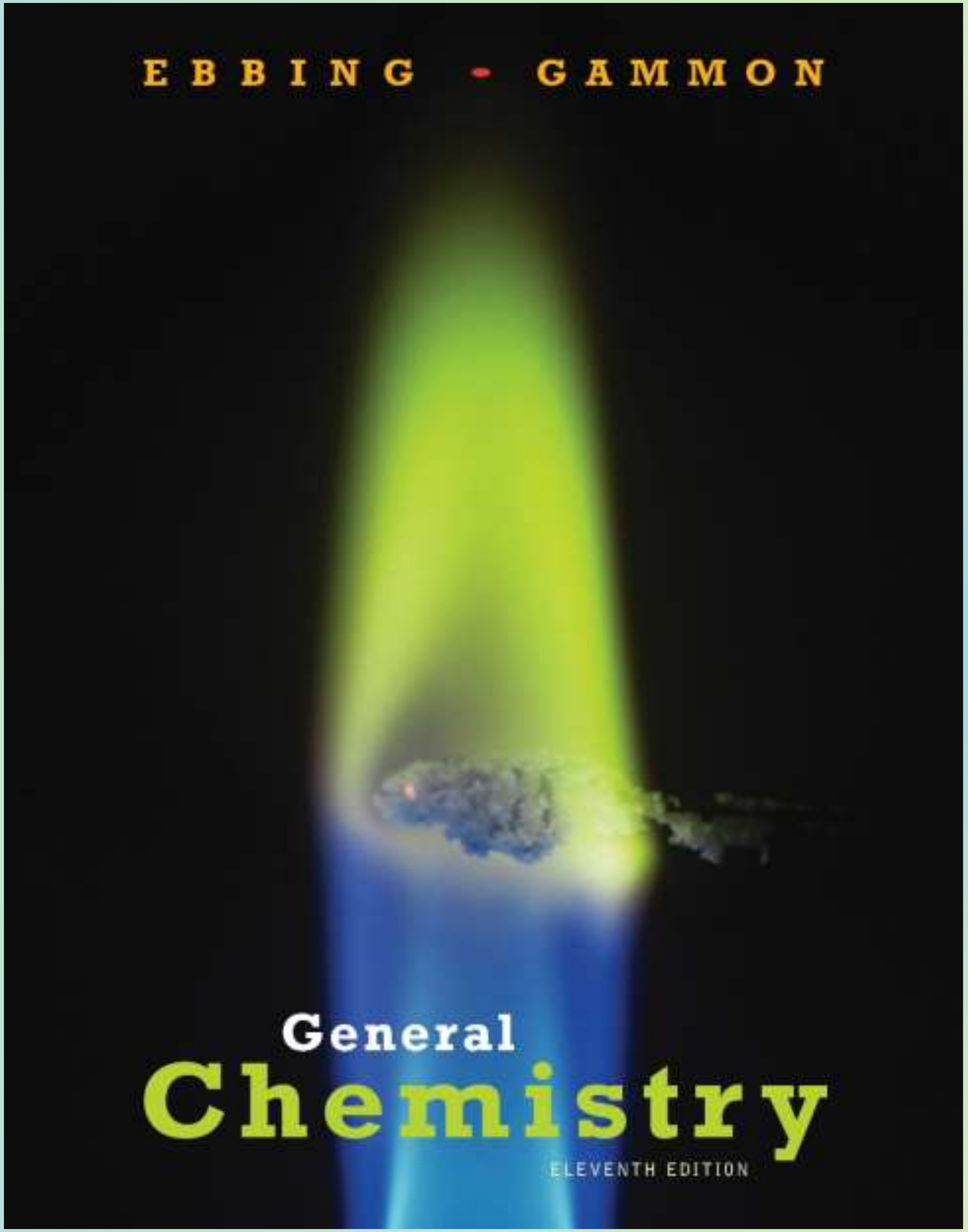


Quantum Theory of The Atom

7.5 Quantum Numbers and Atomic Orbitals:

- Quantum mechanics: each electron in an atom is described by four different quantum numbers, three of which (n, l, and m_l) specify the wave function that gives the **probability** of finding the electron at various points in space.

- Three different quantum numbers are needed because there are three dimensions to space.

- Wave function for electron in an atom is called an atomic orbital

- Atomic orbital has a definite shape and can be **qualitatively** described by the region of space where there is high probability of finding the electrons.

- The fourth quantum number (m_s) refers to a magnetic property of electrons called spin.

- ✓ 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)

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

- ✓ Smaller n → lower energy.
- ✓ n can have **any positive value: 1, 2, 3, and so on**

Letter	*K*	*L*	*M*	*N* . . .
n	1	2	3	4 . . .

- ✓ In H atom or single-electron atomic ions (Li^{2+} and He^{+}) *n* is the only quantum number determining the energy
- ✓ For other atoms, the energy also depends slightly on *l* quantum number.
- ✓ (For a given n, energy of an orbital increases with *l* value.

- ✓ Larger *n* value → larger orbital size.
- ✓ Orbitals with same *n* value belong to the same **shell**.

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 . . .

- ✓ Orbitals of the same *n* but different *l* belong to different *subshells* of a given shell.
- ✓ Within each shell of quantum number n, there are *n* different kinds of orbitals.
- ✓ (s, p, d, f, ..) have distinctive shapes
- ✓ Example: M shell (*n* = 3) → 3 kinds of orbitals
- ✓ (*n* = 3) → possible values for *l* are 0 (*s*), 1 (*p*), and 2 (*d*)
- ✓ Letter symbols of *l* quantum numbers → spectroscopic terminology (describing the lines in a spectrum as:
  sharp, **p**rincipal, **d**iffuse, and **f**undamental
- ✓ 2*p* → a subshell with quantum numbers *n* = 2 and *l* = 1.

3. Magnetic Quantum Number (m_l)

This quantum number distinguishes orbitals of given n and l, 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*.
- ✓ For *l* = 0 (s subshell), the allowed m_l quantum number is 0 only
- ✓ For *l* = 1 (p subshell), m_l = −1, 0, and +1
- ✓ Note : There are three different orbitals in the p subshell with the same shape but different orientations in space.
- ✓ All orbitals of a given subshell have the same energy.

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

- ✓ An electron spins on its axis → Circulating electric charge that generates a magnetic field.
- ✓ An electron behaves like a small bar magnet, with a north and a south pole

(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.

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

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

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

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

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

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*s*	1
2	0	0	2*s*	1
2	1	−1, 0, +1	2*p*	3
3	0	0	3*s*	1
3	1	−1, 0, +1	3*p*	3
3	2	−2, −1, 0, +1, +2	3*d*	5
4	0	0	4*s*	1
4	1	−1, 0, +1	4*p*	3
4	2	−2, −1, 0, +1, +2	4*d*	5
4	3	−3, −2, −1, 0, +1, +2, +3	4*f*	7

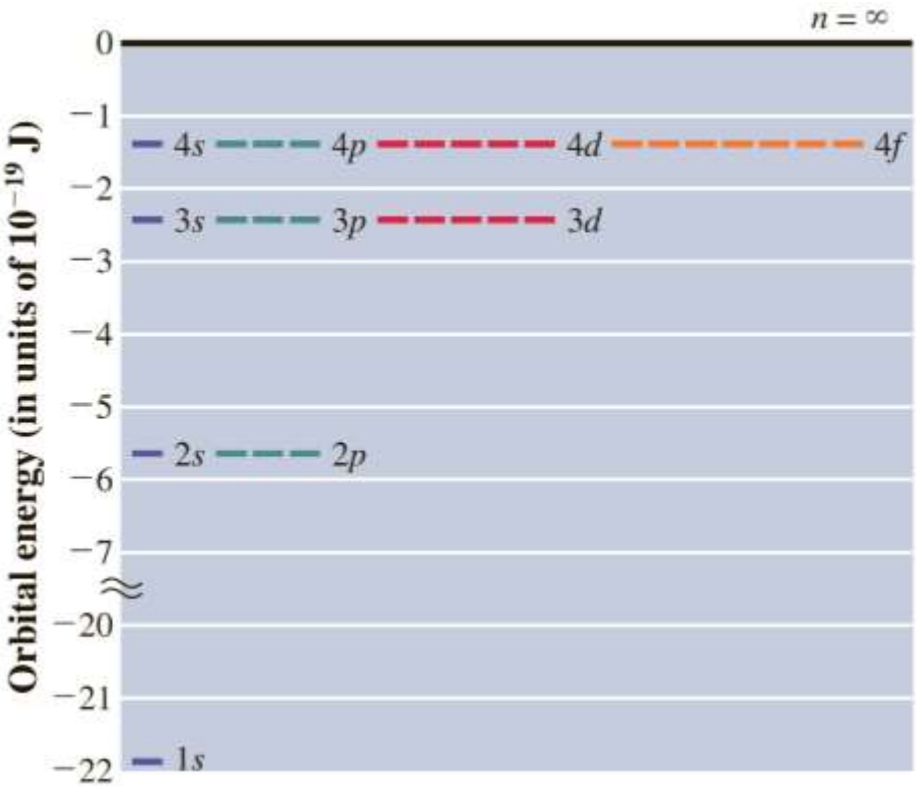
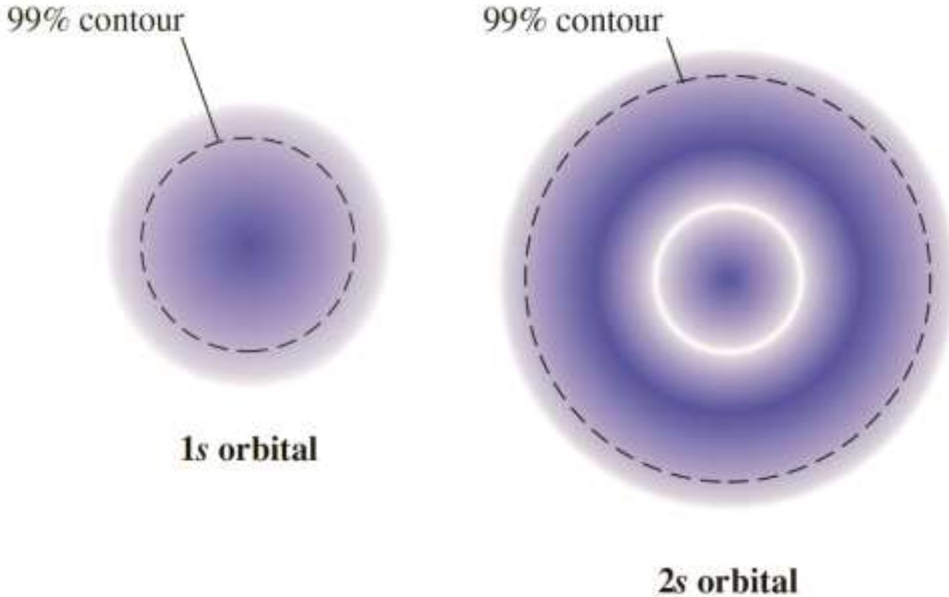
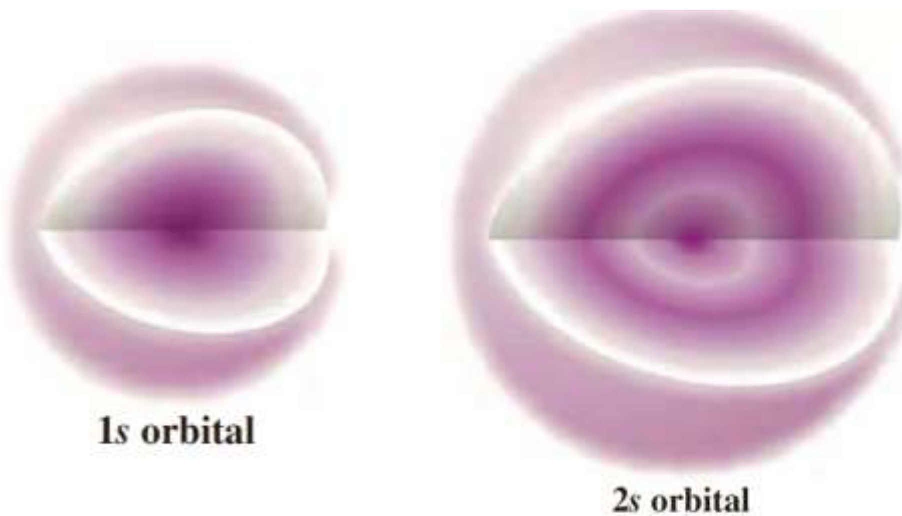


Figure 7.21 ▲

Orbital energies of the hydrogen atom The lines for each subshell indicate the number of different orbitals of that subshell. (Note break in the energy scale.)



Cross-sectional representations of the probability distributions of *s* orbitals In a 1*s* orbital, the probability distribution is largest near the nucleus. In a 2*s* orbital, it is greatest in a spherical shell about the nucleus. Note the relative "size" of the orbitals, indicated by the 99% contours.



Cutaway diagrams showing the spherical shape of *s* orbitals In both diagrams, a segment of each orbital is cut away to reveal the electron distribution of the orbital.

Atomic Orbital Shapes