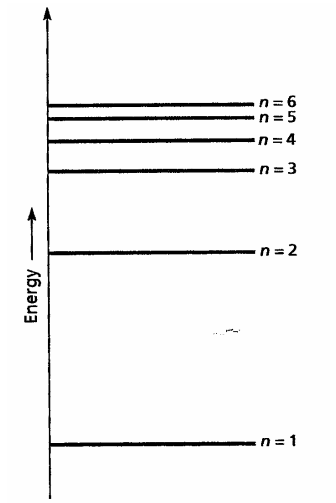
THE 4 QUANTUM NUMBERS (n, l, m_l, m_s)

THE PRINCIPAL QUANTUM NUMBER (n)

- Designates the main energy level (floor) or shell.
- Values: 1, 2, 3, …….∞. n = 7 is the highest number of shell used for the atoms known.
- Describes the **CLOUD SIZE**. The larger the value of n, the larger the cloud size.
- Energy levels closer to the nucleus have lower energy. As n increases, the orbital becomes larger and the electron spends more time farther from the nucleus. An increase in n also means that the electron has a higher energy and is therefore less tightly bound to the nucleus.
- The larger n is, the greater the average distance of an electron in the orbital from the nucleus and therefore the larger (and less stable) the orbital.
  The maximum number of electrons possible in a given shell is $2n^2$.



The main energy levels of an atom are represented by the principal quantum number, n.

LEVEL	MAXIMUM NO. OF ELECTRONS $2n^2$
n = 1	2
n = 2	8
n = 3	18
n = 4	32
n = 5	50
n = 6	72
n = 7	98

In reality there are only 32 electrons in levels 5, 6, and 7 because of the number of different elements discovered or man-made.

ANGULAR MOMENTUM QUANTUM NUMBER (l)

- Designates the sub-level (apartment) where the electron can be found.
- Gives the **SHAPE OF THE ORBITALS**.
- Values of l: from 0 to (n-1) for each value of n.
- The value of l for a particular orbital is generally designated by the letters *s*, *p*, *d*, and *f* corresponding to l values of 0., 1, 2, and 3. for the known atoms, only *s, p, d*, and *f* exist.

Value of l	**0**	**1**	**2**	**3**	4	5
Sub-level	*s*	*p*	*d*	*f*	*g**	*h**

*These sublevels are not used in the ground state of any known element.

- Each sublevel is given a letter designation (like s) and a number designation (s = 0). This allows you to put these two quantum numbers together to identify the shape and location of the atomic orbital.(1s, 4f, 3d etc.)

MAGNETIC QUANTUM NUMBER (m_l)

- Designates the orbital (room) where the electron can be found.
- Gives the **DIRECTION IN SPACE** that the orbital takes.
- m_l specifies to which orbital within a subshell the electron is assigned. Orbitals in a given subshell differ only in their orientation in space, not in their shape.
- Values of m_l: from $-l$, ….0, ….$+l$.
- The middle orbital of a subshell has a value of 0. Orbitals to the left of the middle orbital have negative numbers; to the right, they have + numbers.

m_l = 0 - -1 0 +1 -2 -1 0 +1 +2 -3 -2 -1 0 +1 +2 +3

l = 0 1 2 3

s subshell *p subshell* *d subshell* *f subshell* *g, h,i, j, etc…..*

TABLE 6.2 △ Relationship Among Values of n, l, and m_l through $n = 4$

n	l	Subshell designation	m_l	Number of orbitals in subshell
1	0	1s	0	1
2	0	2s	0	1
	1	2p	1, 0, −1	3
3	0	3s	0	1
	1	3p	1, 0, −1	3
	2	3d	2, 1, 0, −1, −2	5
4	0	4s	0	1
	1	4p	1, 0, −1	3
	2	4d	2, 1, 0, −1, −2	5
	3	4f	3, 2, 1, 0, −1, −2, −3	7

SPIN QUANTUM NUMBER (m_s)

- Designates the **SPIN OF THE ELECTRON** and describes the behavior of the electron, not the location.
- Values: +½ , -½.
- Arrow up ↑ is +½, (referred to as "spin up"); arrow down ↓ is –½ (referred to as "spin down".

SHAPES OF ATOMIC ORBITALS

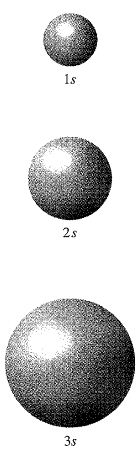
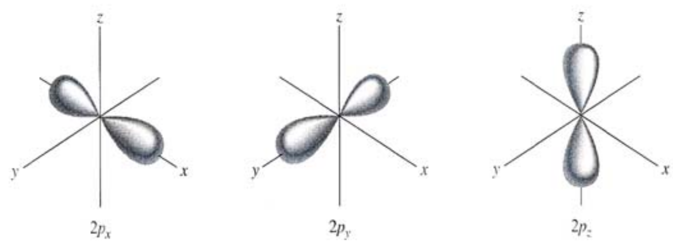
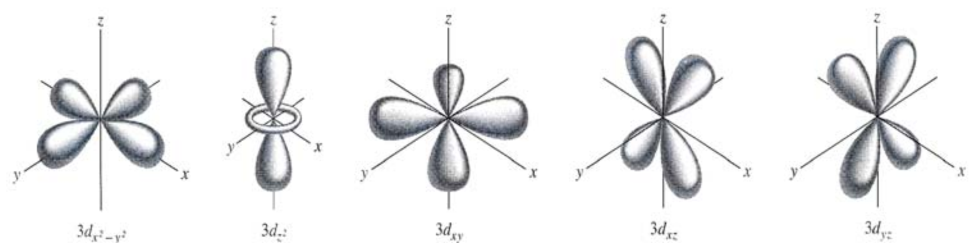


FIGURE 6.19 Contour representations of the 1s, 2s, and 3s orbitals. The relative radii of the spheres correspond to a 90 percent probability of finding the electron within each sphere.

FIGURE 7.19 The boundary surface diagrams of the three 2p orbitals. These orbitals are identical in shape and energy, but their orientations are different. The p orbitals of higher principal quantum numbers have a similar shape.





Boundary surface diagrams of the five 3d orbitals. Although the $3dz^2$ orbital looks different, it is equivalent to the other four orbitals in all other respects. The d orbitals of higher principal quantum numbers have similar shapes.

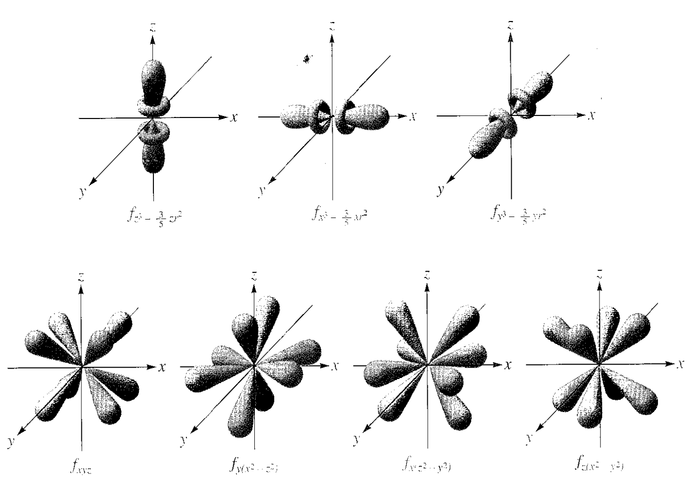
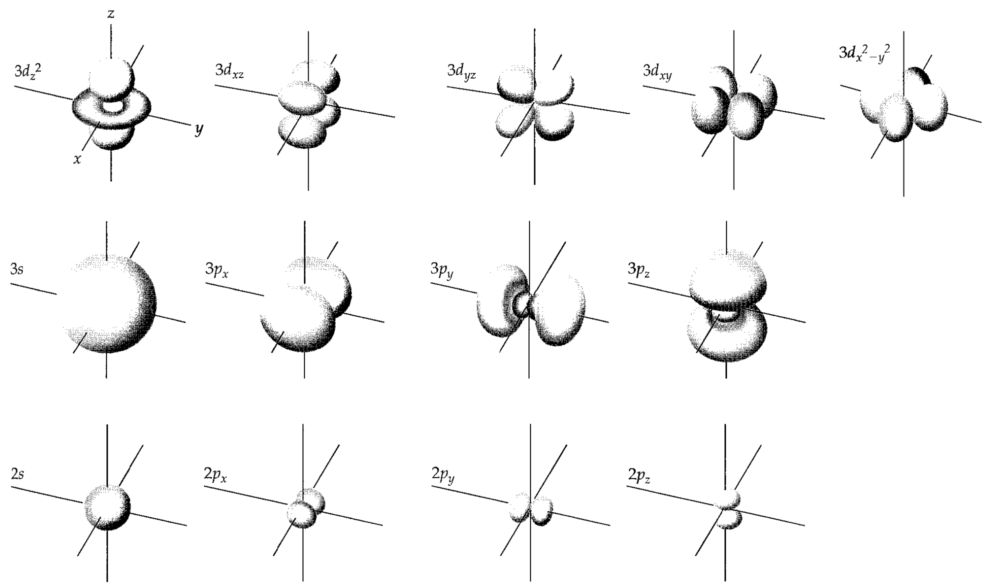


Figure 7.17
Representation of the 4f orbitals in terms of their boundary surfaces.



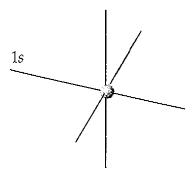


Figure 7.17 Boundary surface diagrams for electron densities of 1*s*, 2*s*, 2*p*, 3*s*, and 3*d* orbitals for a hydrogen atom. For the *p* orbitals the subscript letter on the orbital notation indicates the cartesian axis along which the orbital lies. The plane passing through the nucleus (perpendicular to this axis) is called a planar node ($\ell = 1$). The *d* orbitals all have two planar nodes ($\ell = 2$). See the text for a description of the notation used to differentiate the *d* orbitals.

SUBLEVEL	VALUE OF *l*	ORBITAL SHAPE
s	0	Spherical (size of s increases as n increases)
p	1	Dumbbell shape; 2 regions of electron density
d	2	4 regions of electron density
f	3	8 regions of electron density

QUESTIONS: (Room here)

1. List the values of n, l, and m_l for orbitals in the 4d subshell.

2. Give the values of the quantum numbers associated with the orbitals in the 3*p* subshell.

3. What is the total number of orbitals associated with the principal quantum number $n = 3$?_____
4. What is the total number of orbitals associated with the principal quantum number $n = 4$?_____
5. What is the maximum number of electrons that can occupy the fourth energy level.. ________
6. When $n = 5$ what are the possible values for l? ________
7. When $l = 2$ what are the possible values of m_l? __________
8. How many sublevels are possible in the third energy level? ___________

9. What is the maximum number of electrons that can occupy a *d* sublevel? _______
10. What is the maximum number of electrons that can occupy *a g* sublevel? __________
11. When $n = 2$, the values of l can be ____ and _____.
12. When $l = 1$, the values of m_l can be ______________________and the subshell has the letter designation of ___________.
13. When a subshell is labeled *s*, the value of l is _____ and m_l has value(s) of ________________.
14. When a subshell is labeled *p*, _________ orbitals occur within the subshell.
15. When a subshell is labeled *f*, there are _____ values of m_l and ______ orbitals occur within the subshell.

THE ENERGIES OF ORBITALS (ORDER OF FILLING ORBITALS WITH ELECTRONS

The relative energy of sublevels will now determine the arrangement of electron in atoms (electrons moving into the apartment block).
The **ground state of an atom** is the state in which the electrons are located in the lowest energy levels and sublevels possible. They can move to higher levels or an exited state if excited by some form of energy (light). Sublevels of energy levels overlap. A 4s subshell has lower energy than a 3d subshell. The effect of the overlap is that the atom is more stable when the 4s sublevel is of lower energy than the 3d sublevel. When drawing orbital diagrams (placing electrons in orbitals of increasing energy), electrons occupy sublevels of the lowest energy.

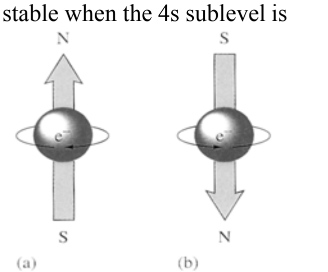


Figure 7.19
A picture of the spinning electron. Spinning in one direction, the electron produces the magnetic field oriented as shown in (a). Spinning in the opposite direction, it gives a magnetic field of the opposite orientation, as shown in (b).

In drawing orbit filling diagrams the following guidelines must be followed:

- THE AUFBAU PRINCIPLE (Building up principle) **ELECTRONS ENTER ORBITALS OF LOWEST ENERGY FIRST.** Electrons are added to atomic orbitals starting with the lowest energy orbital and building up to higher energy orbitals.

- PAULI EXCLUSION PRINCIPLE – **ONLY 2 ELECTRONS CAN OCCUPY AN ORBITAL AND THEY MUST HAVE OPPOSITE SPINS.** No two electrons in an atom can have the same four quantum numbers. This means that electrons occupying the same orbital cannot have the same spin. (no 2 electrons can be in the same place at the same time).

↑↓	↑↑
THIS	**NOT THIS:**

- HUND'S RULE: **WHEN ELECTRONS OCCUPY ORBITALS OF EQUAL ENERGY, ONE ELECTRON ENTERS EACH ORBITAL UNTIL ALL THE ORBITALS CONTAIN ONE ELECTRON WITH SPINS PARALLEL.** The most stable arrangement of electrons in subshells is the one with the greatest number of parallel spins, without violating the Pauli Exclusion Principle. (Electrons occupy orbitals in a sublevel one at a time until each orbital has 1 electron. They will not double up until each orbital has at least one electron.)

[↑][↑][↑]	[↑][↓][↑]	[↑↓][↑][ ]
THIS	**NOT THIS**	**NOT THIS**

****NOTE:** Orbitals in the same subshell are of equal energy so an electron may occupy any of the orbitals in that subshell with equal probability. This means that the first orbital on the left is not necessarily the first one filled. By convention, we use this as the first orbital filled. Also the first electron in a sublevel may be spin up ↑ or spin down ↓ with equal probability. We designate the first electron to be spin up ↑ by convention. Once the first one in has a spin, ↑ or ↓ the remaining 1st electrons in an orbital must have the same spin according to Hund's Rule.

- **All these are of equal probability**
-
:

[↑][↑][ ]	[↑][ ][↑]	[ ][↑][↑]
[↓][↓][ ]	[↓][ ][↓]	[ ][↓][↓]

- **These are not correct.**

[↑][↓][ ]	[↓][↑][ ]	[↑][ ][↓]
[↑][↑][↓]	[↓][↓][↑]	[↑][↓][↑]

ORDER OF FILLING SUBLEVELS

- The Diagonal Rule can be used to determine which order the sublevels fill. (shown below). A better way to do it is to use the periodic table.

In using the periodic table:

- Period numbers are the level number.
- Go from left to write. Designate each period and sublevel ex. 2p, 3f
- Sublevel *d* is one level lower than the main energy level.
- Sublevel *f* is two levels lower than the main energy level.

ORDER 1s 2s 2p 3s 3p 4s 3d 4p 5s 4d 5p 6s 4f 5d 6p 7s 5f 6d 7p

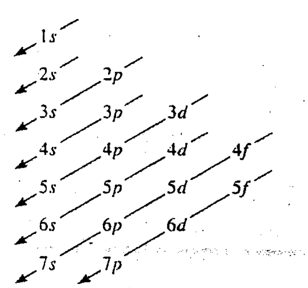
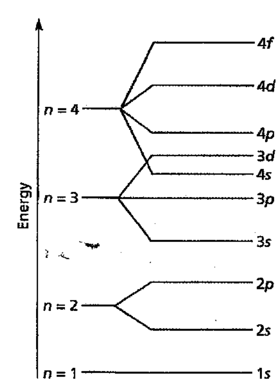


FIGURE 7.23 *The order in which atomic subshells are filled in a many-electron atom. Start with the 1s orbital and move downward, following the direction of the arrows. Thus the order goes as follows: 1s < 2s < 2p < 3s < 3p < 4s < 3d < . . . .*



The direction of the arrow indicates the order in which atomic orbitals are filled according to the Aufbau principle.

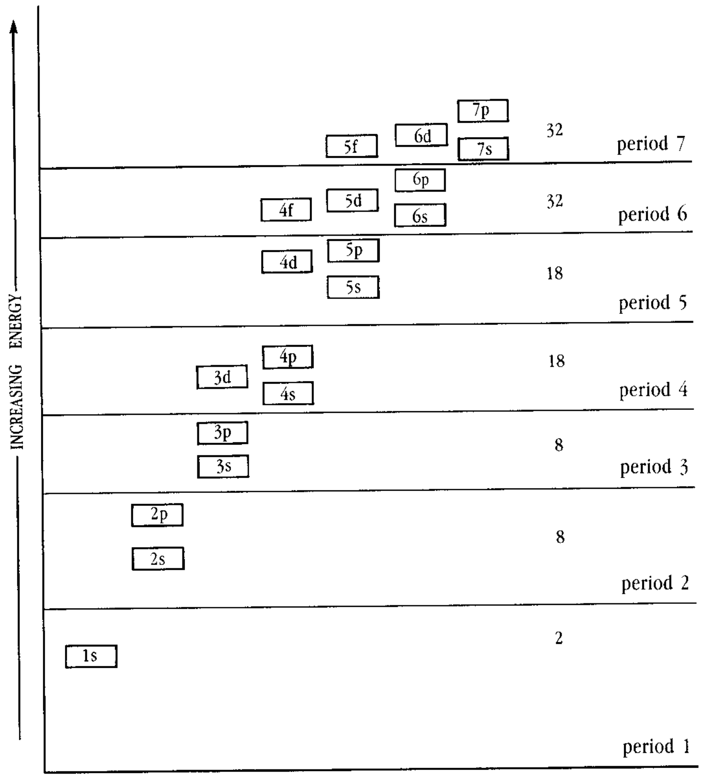
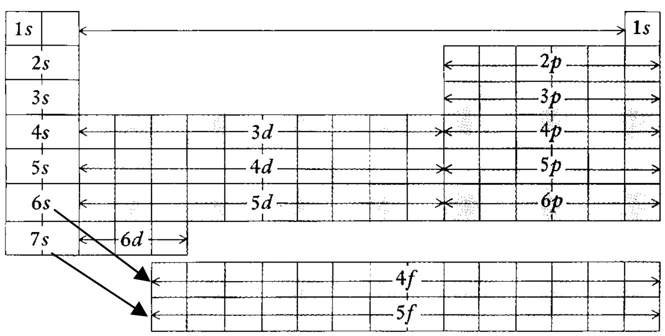
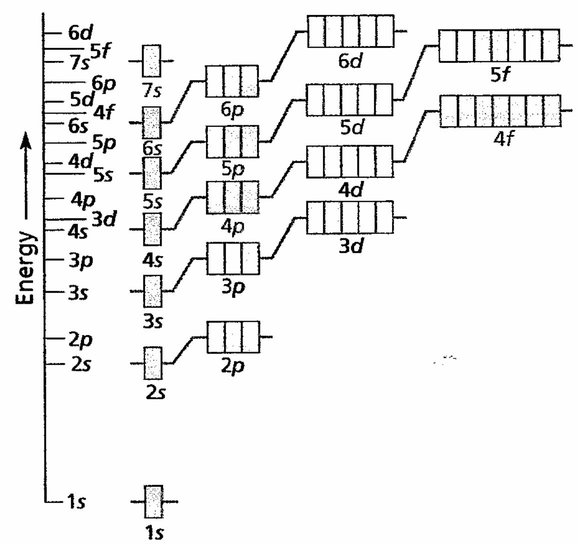


Figure
The elements in each period correspond to the order of filling of the sublevels shown.

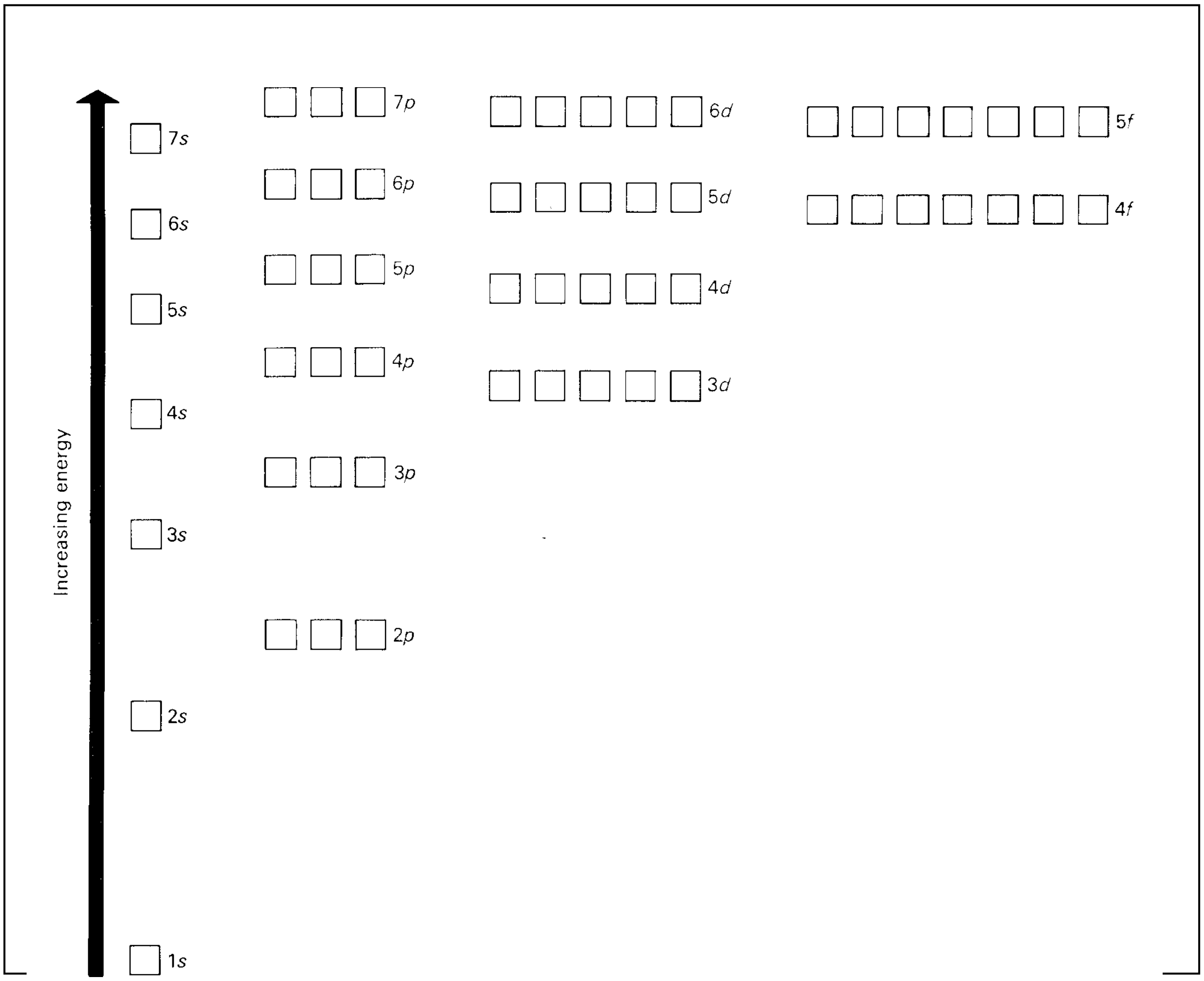


s–block elements   d–block elements (transition metals)
p–block elements   f–block elements: lanthanides (4f) and actinides (5f)



The order of increasing energy for atomic sublevels is shown on the vertical axis. Each individual box represents an orbital.

Use the following energy diagrams to draw the orbital filling diagrams for the berkelium atom (#97)
****USE YOUR TEST COPY OF THE PERIODIC TABLE.**



Ex: An oxygen atom has a total of eight electrons. Write the 4 quantum numbers for each of the eight electrons in the ground state. Note the configuration of $2p^4$ which means the $2p$ sublevel has 4 electrons.

The orbital diagram is:

↑↓	↑↓	↑↓ ↑ ↑
$1s^2$	$2s^2$	$2p^4$

Electron	*n*	*l*	m_l	m_s	orbital
1	1	0	0	+½	1*s*
2					
3					
4					
5	2	1	-1	+½	2*p*
6					
7					
8					

<u>PROBLEMS – LOT OF PRACTICE</u>

1. For the following sets of quantum numbers for electrons, indicate which quantum numbers n, l, m_l **could not** occur and state why.
   (a) 3, 2, 2 (b) 2, 2, 2 (c) 2, 0, -1

2. Which of the following sets of quantum numbers **are not allowed** for describing an electron in an orbital?

	n	l	m_l	m_s
a.	3	2	-3	+½
b.	2	3	0	-½
c.	2	1	0	-½

3. Which choice is a possible set of quantum numbers for the last electron added to make up an atom of gallium Ga in its ground state?

	n	l	m_l	m_s
a.	4	2	0	-½
b.	4	1	0	+½
c.	4	2	-2	-½
d.	3	1	+1	+½
e.	3	0	0	-½

4. Which of the following are incorrect designations for an atomic orbital?
   (a) 3*f* (b) 4*s* (c) 2*d* (d) 4*f*

5. How many orbitals in an atom can have the following designations?
   (a) 2s (b) 3*d* (c) 4*p* (d) $n = 3$

6. For each of the following give the subshell designation, the m_l values, and the number of possible orbitals.
   (a) $n = 3$ $l = 2$ (b) $n = 4$ $l = 3$ (c) $n = 5$ $l = 1$

7. Identify the atoms whose last electron is represented by the set of quantum numbers below:

	n	l	m_l	m_s
a.	3	1	0	+½
b.	5	3	+2	-½
c.	2	0	0	+½
d.	3	2	-2	-½
e.	4	1	+1	-½

8. What is the subshell designation for each of the following cases
   (a) $n = 2,\ l = 0$
   (b) $n = 4,\ l = 2$
   (c) $n = 5,\ l = 1$
   (d) $n = 3,\ l = 2$
   (e) $n = 4,\ l = 3$

9. The quantum numbers listed below are for four different electrons in the same atom. Arrange them in order of increasing energy. Indicate whether any two have the same energy.
   (a) $n = 4$, $l = 0$ $m_l = 0$ $m_s = +½$
   (b) $n = 3$, $l = 2$ $m_l = 1$ $m_s = +½$
   (c) $n = 3$, $l = 2$ $m_l = -2$ $m_s = -½$
   (d) $n = 3$, $l = 1$ $m_l = 1$ $m_s = -½$

DO ASSIGNMENT #3 ON ASSIGNMENT SHEET
P. 340-342 #20, 59-62, 65, 67, 68, 70, 72.