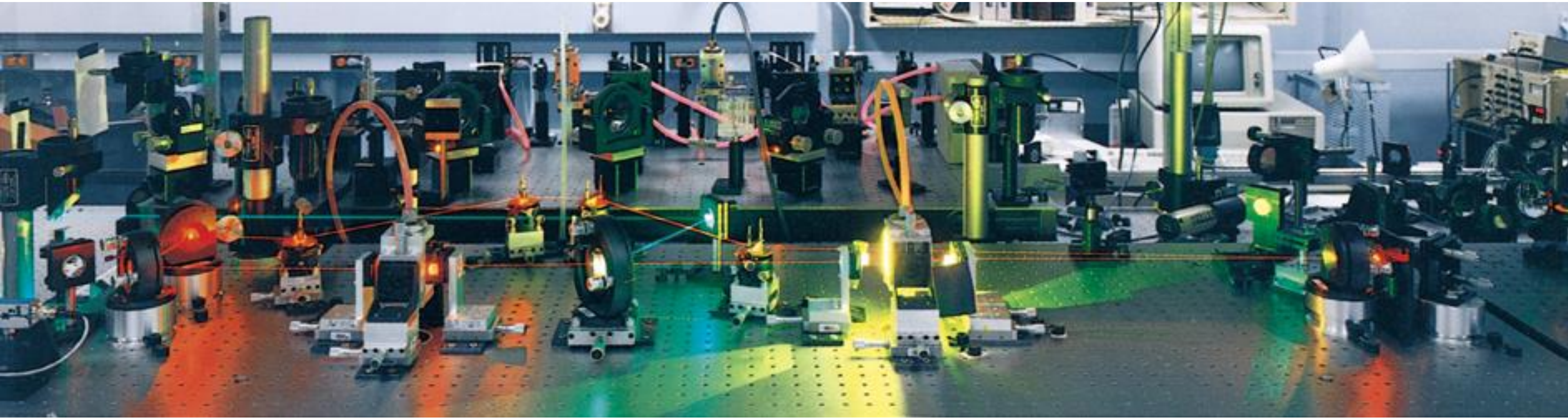


Quantum Theory and the Electronic Structure of Atoms

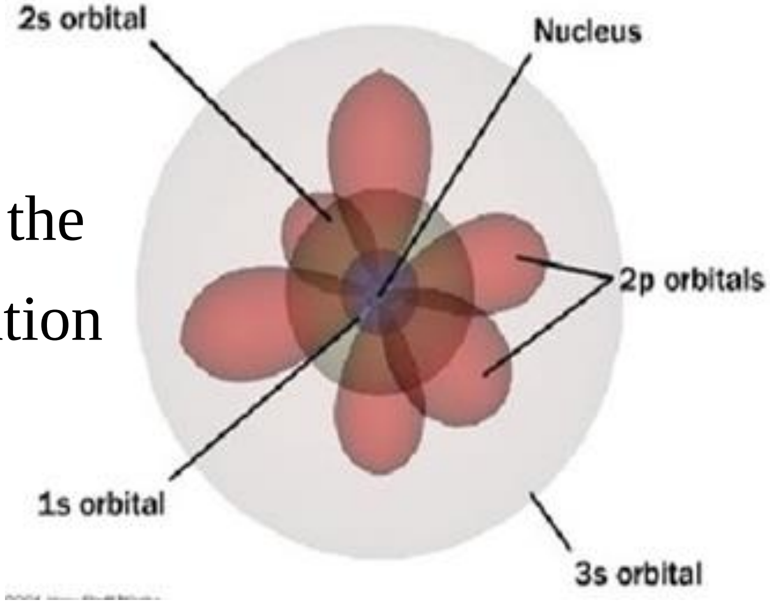
Quantum numbers

Quantum numbers are used to differentiate between electrons

i. In quantum theory, each electron in an atom is assigned a set of four quantum numbers.

ii. Three of these give the location of the electron, and the fourth gives the orientation of the electron within the orbital

iii. Definitions of numbers

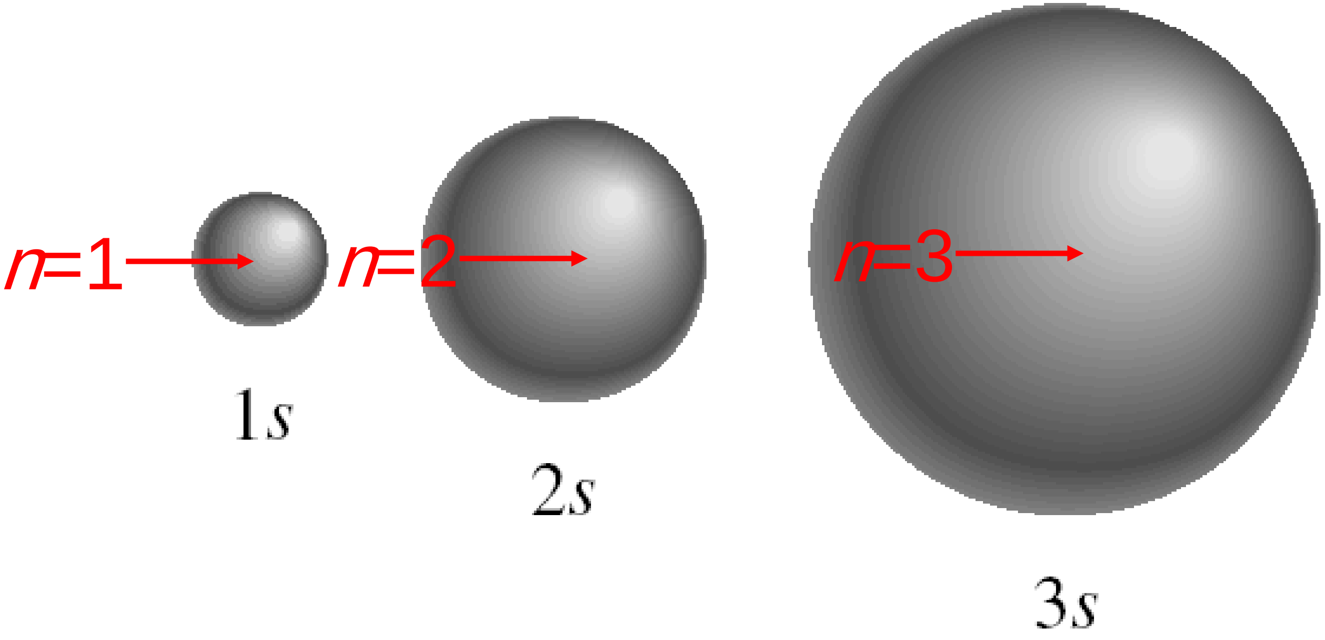


quantum numbers (n, l, m_l, m_s)

principal quantum number n

n = 1, 2, 3, 4, ….

$\boxed{\text{distance of } e^- \text{ from the nucleus}}$



quantum numbers: (n, l, m_l, m_s)

angular momentum quantum number l

for a given value of n, $l = 0, 1, 2, 3, \ldots n-1$

$n = 1$, $l = 0$

$n = 2$, $l = 0$ **or** 1

$n = 3$, $l = 0, 1,$ **or** 2

$l = 0$ *s* orbital

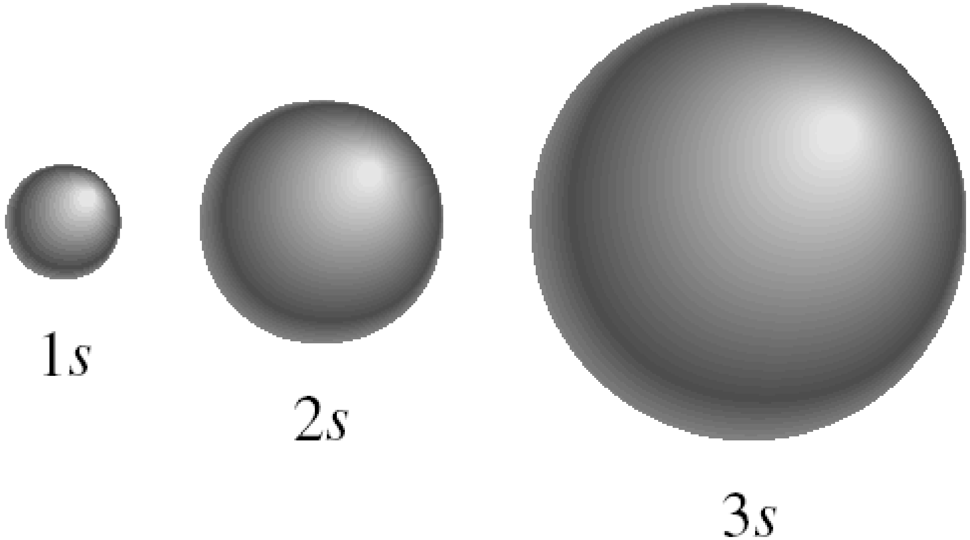
$l = 1$ *p* orbital

$l = 2$ *d* orbital

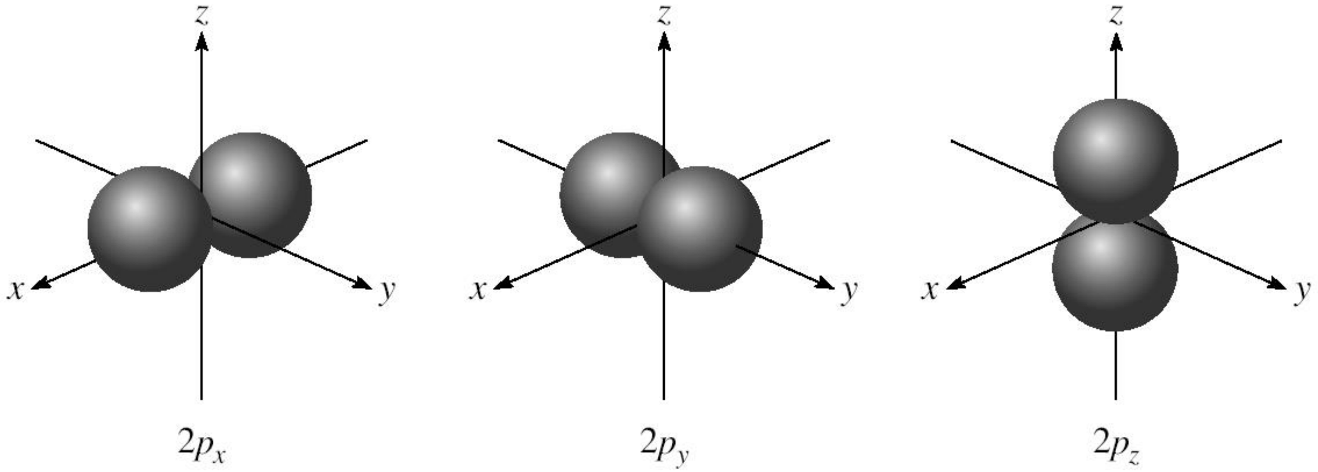
$l = 3$ *f* orbital

Shape of the "volume" of space that the e^- occupies

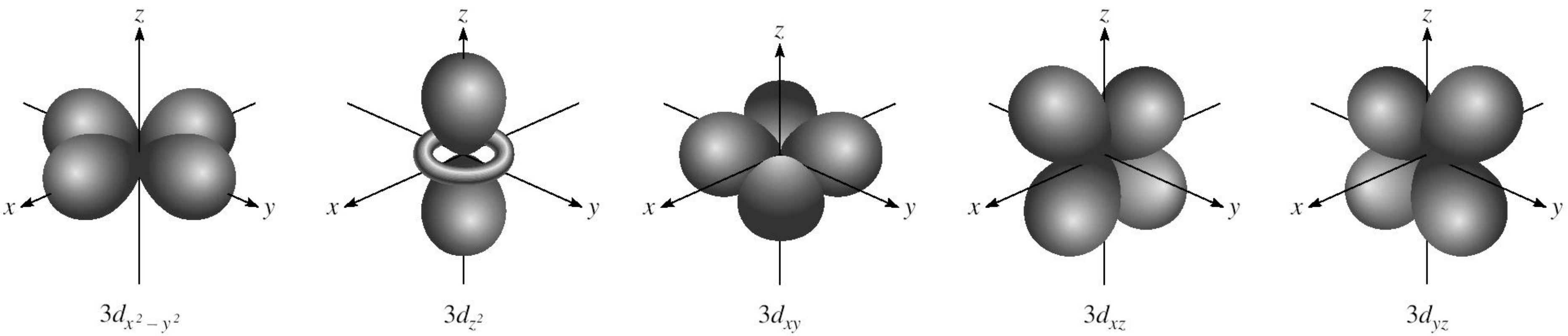
l = 0 (*s* orbitals)



l = 1 (*p* orbitals)



l = 2 (d orbitals)



quantum numbers: (n, l, m_l, m_s)

magnetic quantum number m_l

for a given value of l

$m_l = -l, \ldots, 0, \ldots +l$

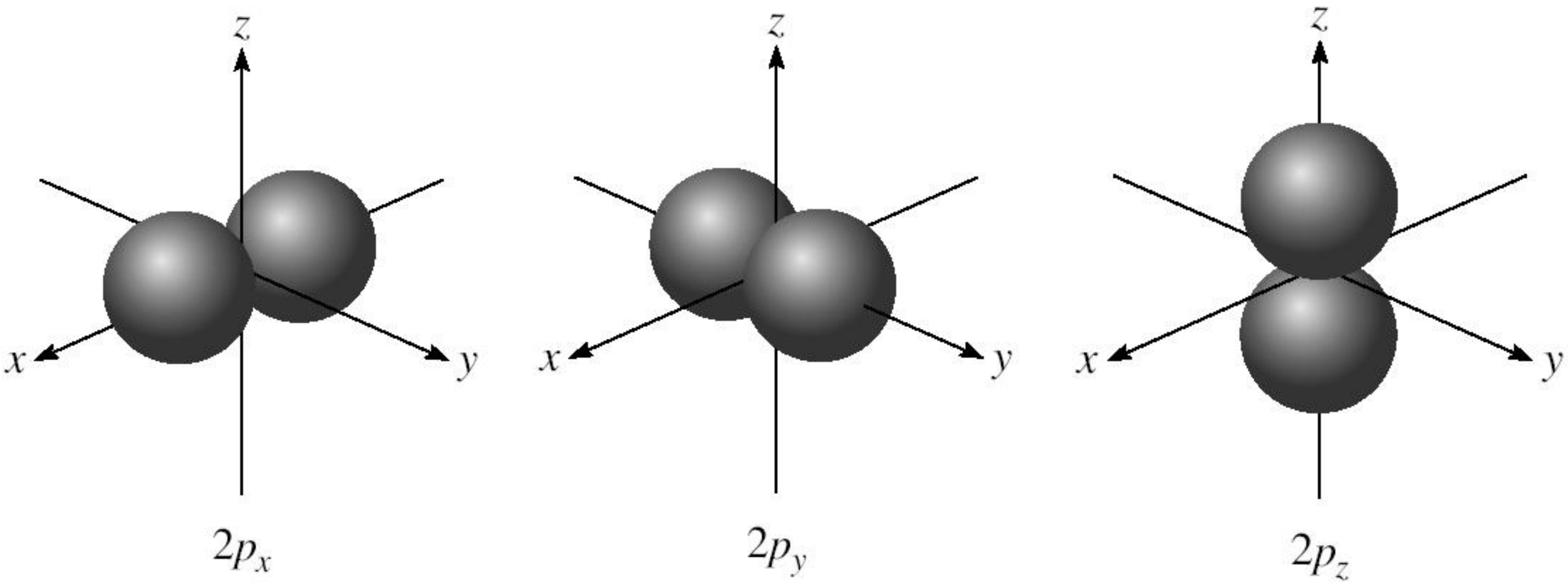
if $l = 1$ (p orbital), $m_l = -1, 0,$ **or** 1

if $l = 2$ (d orbital), $m_l = -2, -1, 0, 1,$ **or** 2

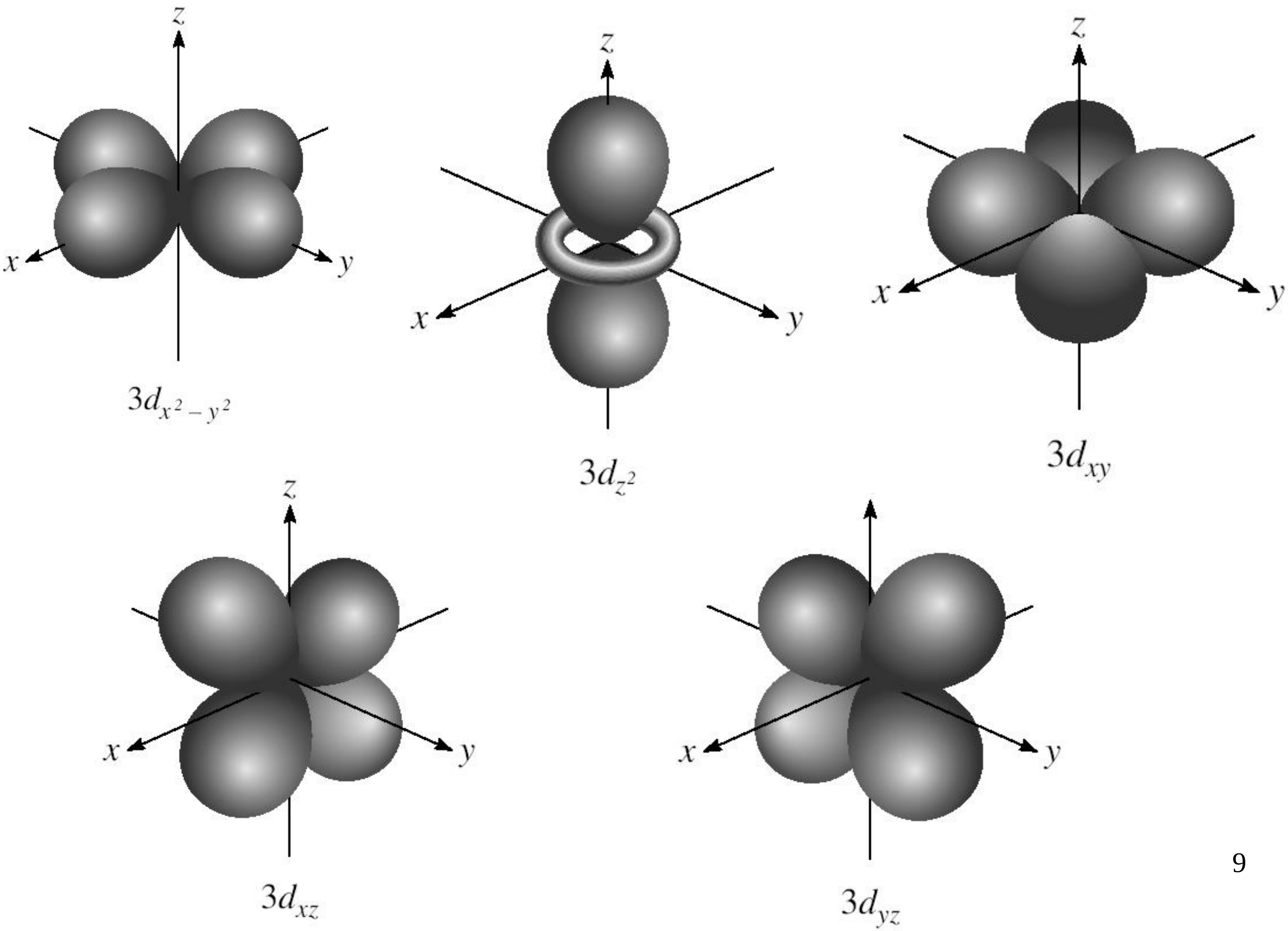
orientation of the orbital in space

m_l = -1, 0, **or** 1

3 orientations is space



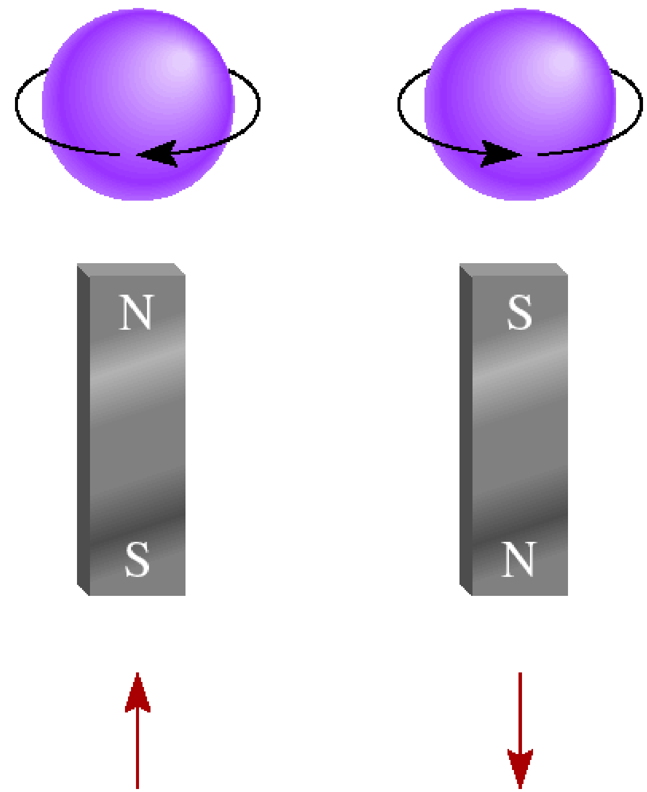
m_l = -2, -1, 0, 1, **or** 2 5 orientations is space



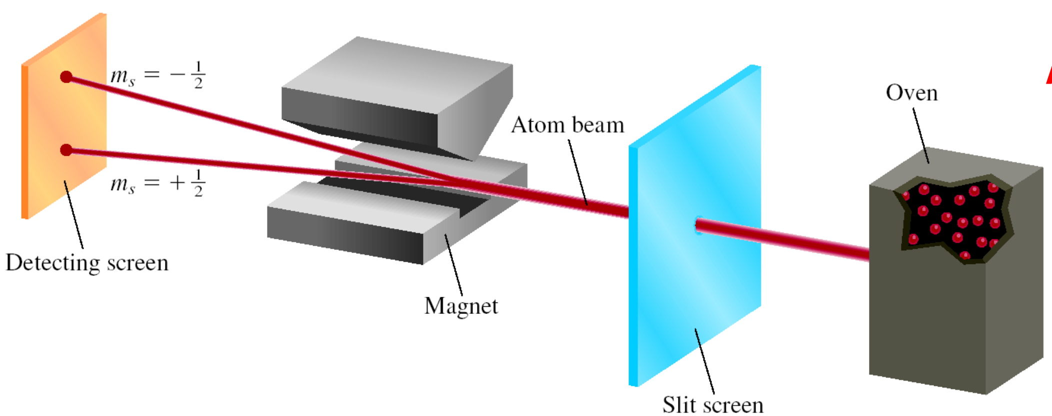
(n, l, m_l, m_s)

spin quantum number m_s

m_s = +½ **or** -½



m_s = +½ m_s = -½



quantum numbers: (n, l, m_l, m_s)

Existence (and energy) of electron in atom is described by its ***unique*** wave function ψ.

Pauli exclusion principle - no two electrons in an atom can have the same four quantum numbers.

Each seat is uniquely identified (E, R12, S8)
Each seat can hold only one individual at a time

TABLE 7.2 Relation Between Quantum Numbers and Atomic Orbitals

n	ℓ	m_ℓ	Number of Orbitals	Atomic Orbital Designations
1	0	0	1	$1s$
2	0	0	1	$2s$
	1	$-1, 0, 1$	3	$2p_x, 2p_y, 2p_z$
3	0	0	1	$3s$
	1	$-1, 0, 1$	3	$3p_x, 3p_y, 3p_z$
	2	$-2, -1, 0, 1, 2$	5	$3d_{xy}, 3d_{yz}, 3d_{xz}, 3d_{x^2-y^2}, 3d_{z^2}$
⋮	⋮	⋮	⋮	⋮

quantum numbers: (n, l, m_l, m_s)

Shell – electrons with the same value of n

Subshell – electrons with the same values of n **and** l

Orbital – electrons with the same values of $n, l,$ **and** m_l

How many electrons can an orbital hold?

If $n, l,$ and m_l are fixed, then $m_s = ½$ or - ½

$\psi = (n, l, m_l, ½)$ or $\psi = (n, l, m_l, -½)$

An orbital can hold 2 electrons

How many 2*p* orbitals are there in an atom?

n=2

↓

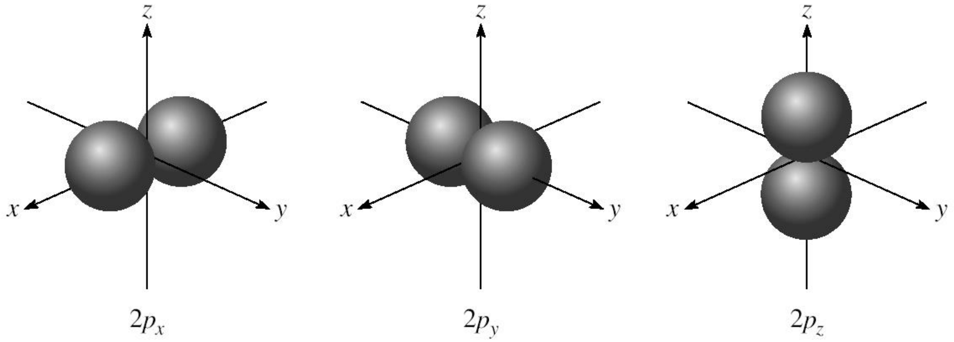
2*p*

↑

l = 1

If l = 1, then m_l = -1, 0, or +1

3 orbitals



How many electrons can be placed in the 3*d* subshell?

n=3

↓

3*d*

↑

l = 2

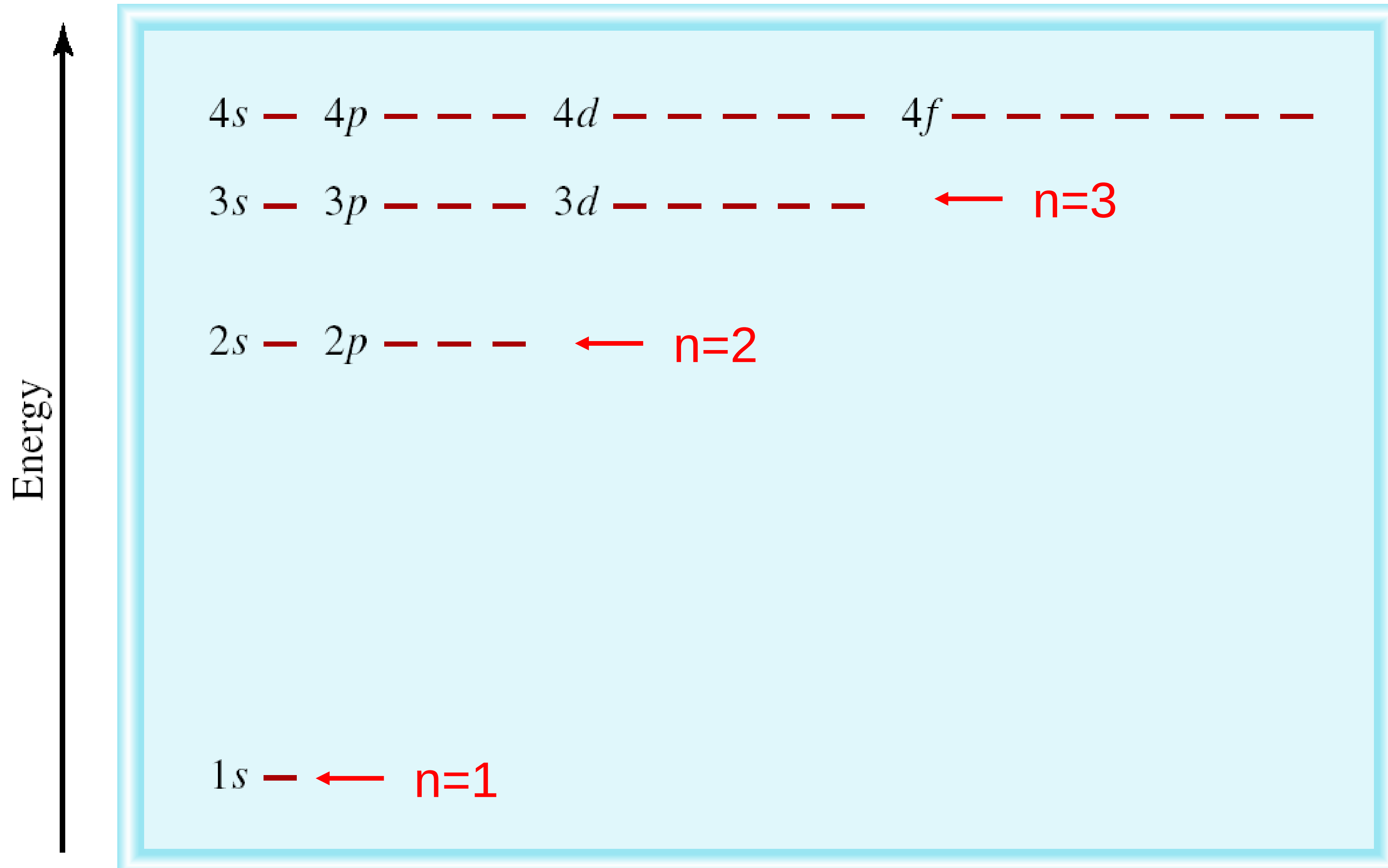
If l = 2, then m_l = -2, -1, 0, +1, or +2

5 orbitals which can hold a total of 10 e^-

The Energies of Orbitals

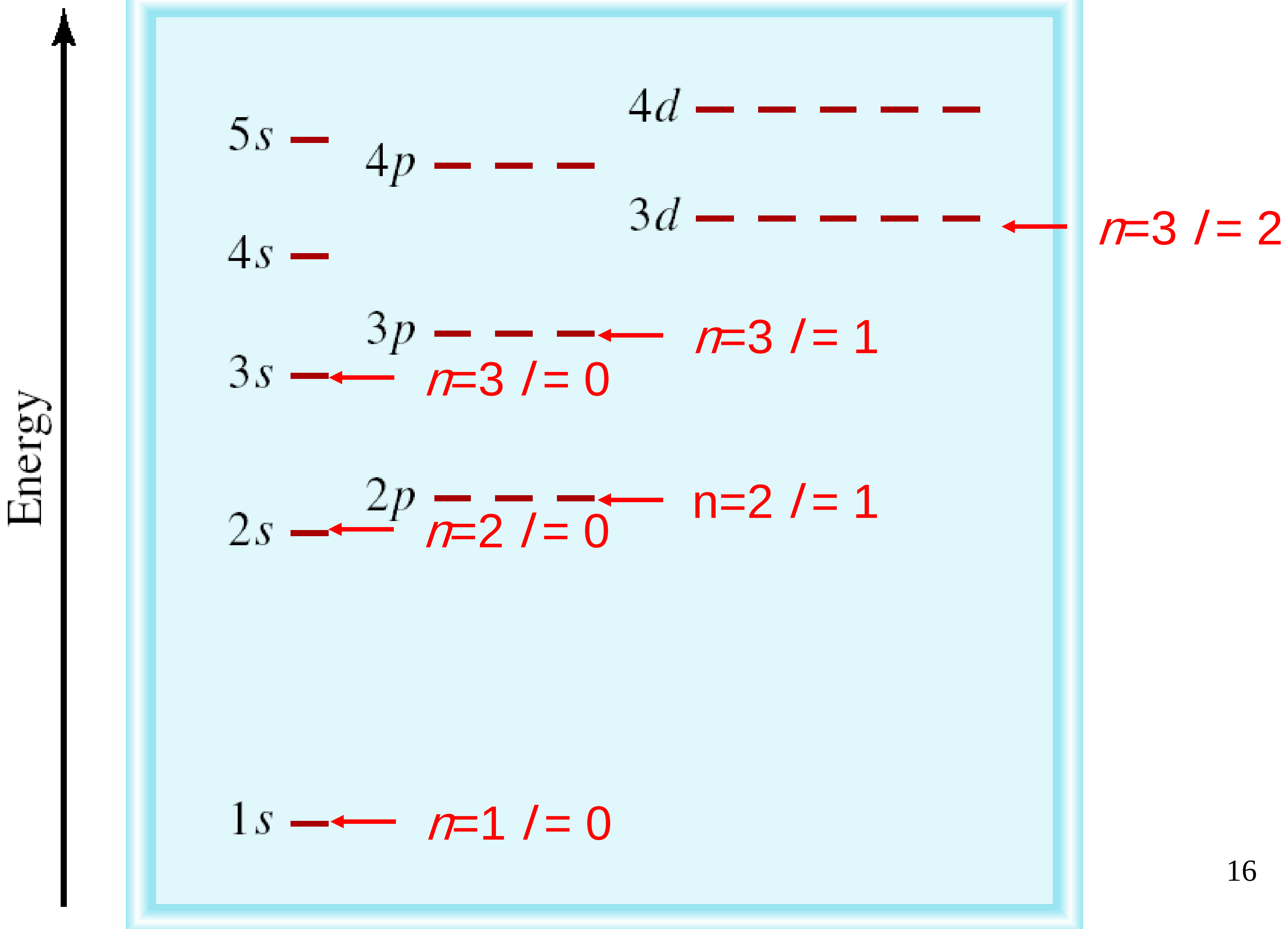
Energy of orbitals in a ***single*** electron atom

Energy only depends on principal quantum number ***n***

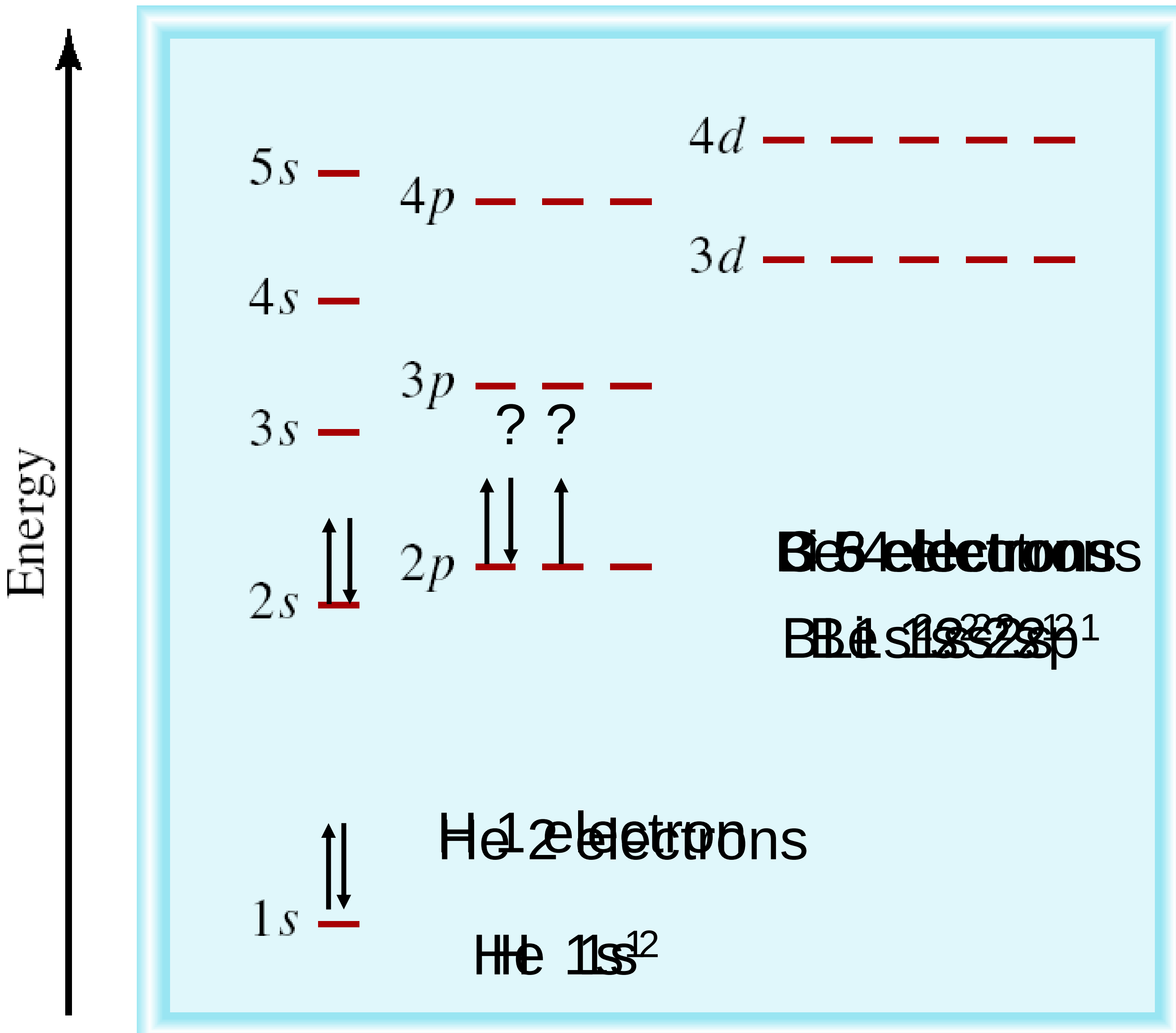


Energy of orbitals in a ***multi***-electron atom

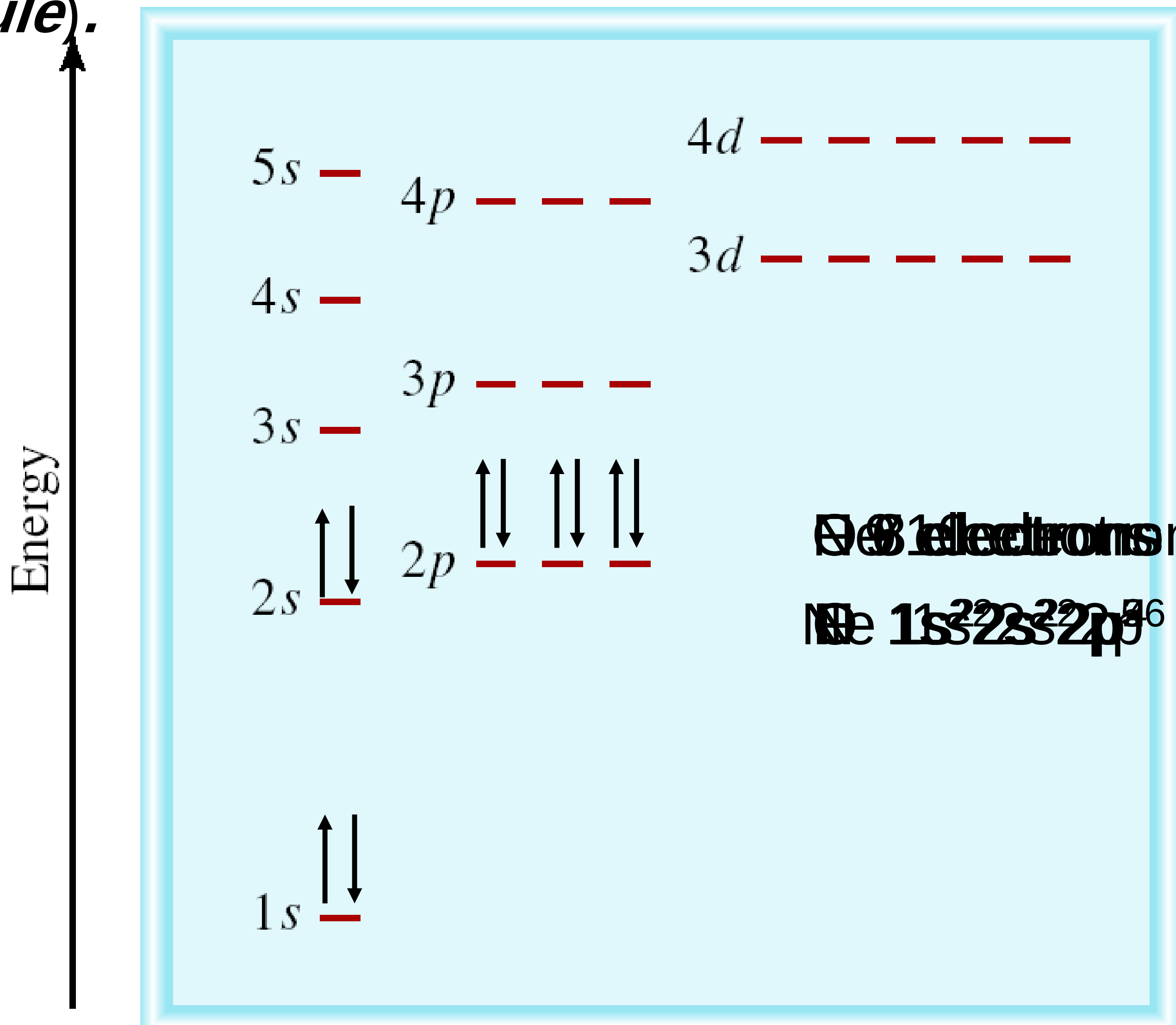
Energy depends on ***n*** and ***l***



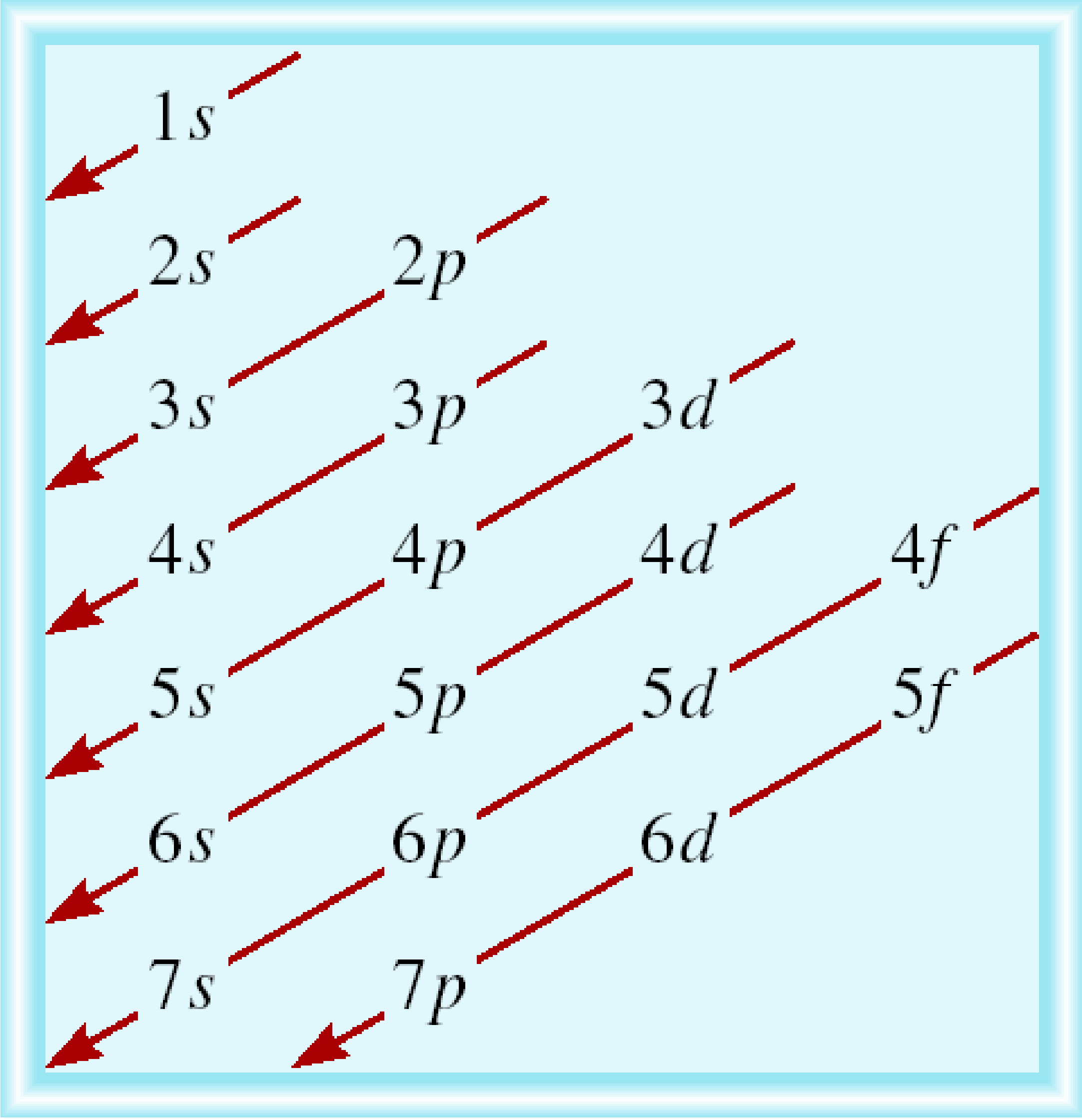
“Fill up” electrons in lowest energy orbitals (***Aufbau principle***)



The most stable arrangement of electrons in subshells is the one with the greatest number of parallel spins (***Hund's rule***).



Order of orbitals (filling) in multi-electron atom



1s < 2s < 2p < 3s < 3p < 4s < 3d < 4p < 5s < 4d < 5p < 6s

Electron configuration is how the electrons are distributed among the various atomic orbitals in an atom.

number of electrons in the orbital or subshell

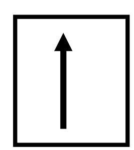
$1s^1$

principal quantum number ***n***

angular momentum quantum number ***l***

Orbital diagram

H



$1s^1$

What is the electron configuration of Mg?

Mg 12 electrons

$1s < 2s < 2p < 3s < 3p < 4s$

$1s^2 2s^2 2p^6 3s^2$ $2 + 2 + 6 + 2 = 12$ electrons

Abbreviated as $[Ne]3s^2$ $[Ne]$ $1s^2 2s^2 2p^6$

What are the possible quantum numbers for the last (outermost) electron in Cl?

Cl 17 electrons $1s < 2s < 2p < 3s < 3p < 4s$

$1s^2 2s^2 2p^6 3s^2 3p^5$ $2 + 2 + 6 + 2 + 5 = 17$ electrons

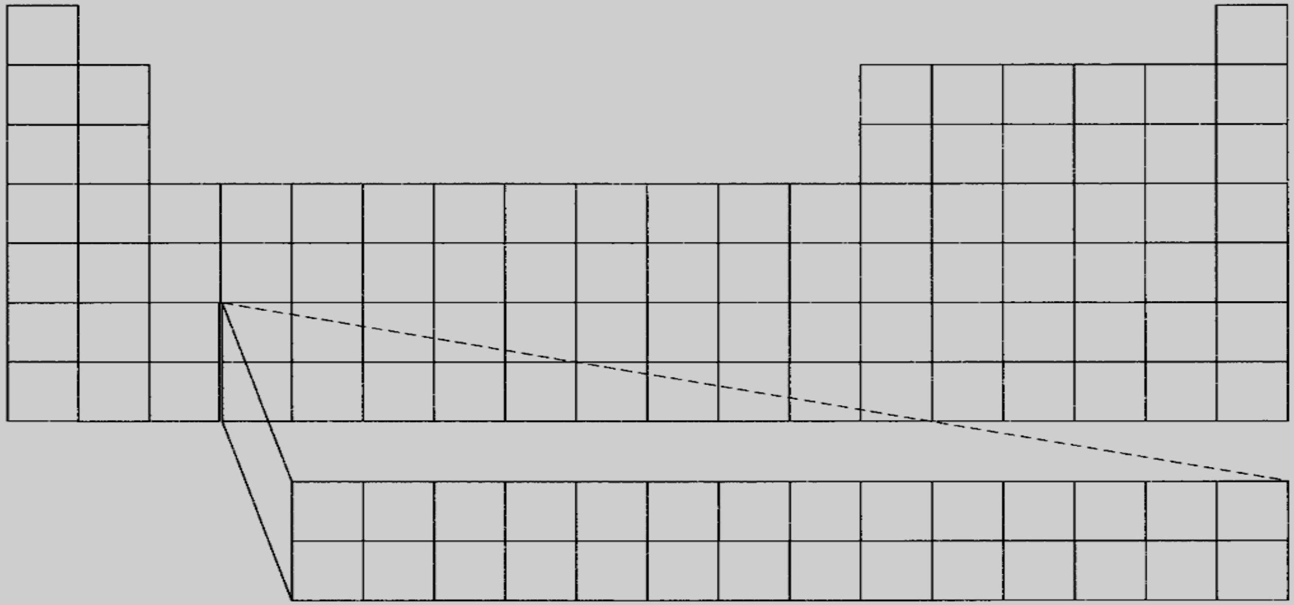
Last electron added to 3p orbital

$n = 3$ $l = 1$ $m_l = -1, 0,$ or $+1$ $m_s = ½$ or $-½$

Distilling Information

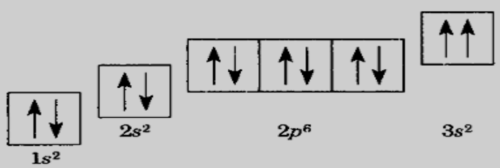
1. Label the *s, p, d,* and *f* blocks in **Table 3-4.**

Table 3-4 Orbital Blocks of the Periodic Table



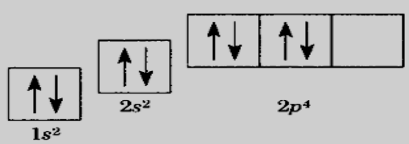
2. **Which guideline, Hund's rule or Pauli's exclusion principle, is violated in the following orbital diagrams?**

a.



a. ______________________________

b.



b. ______________________________

3. **List the element represented by each of the following electron configurations.**

a. $1s^2 2s^2 2p^6 3s^1$ ______________

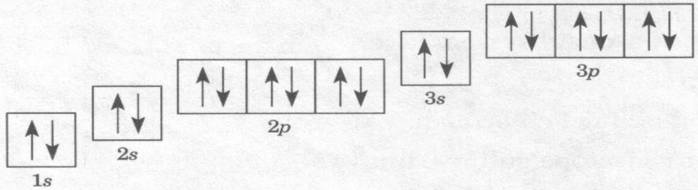
b. $1s^2 2s^2 2p^6 3s^2 3p^6 4s^2 3d^6$ ______________

c. $1s^2 2s^2 2p^6 3s^2 3p^6 4s^2 3d^{10} 4p^6 5s^2 4d^1$ ______________

d. [Rn] $7s^2 5f^2 6d^1$ ______________

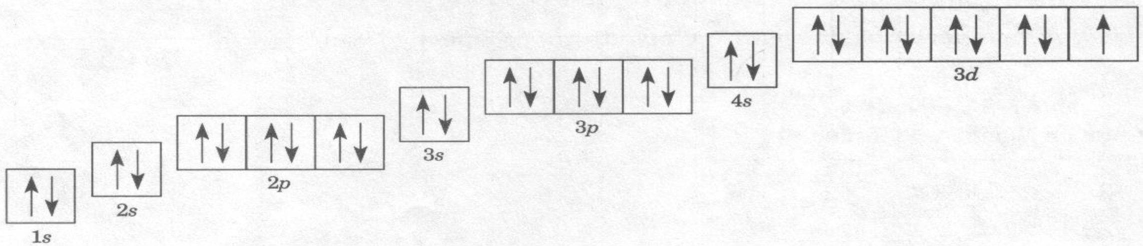
e. [Kr] $5s^2 4d^{10} 5p^4$ ______________

4. **List the element represented by each of the following orbital diagrams.**



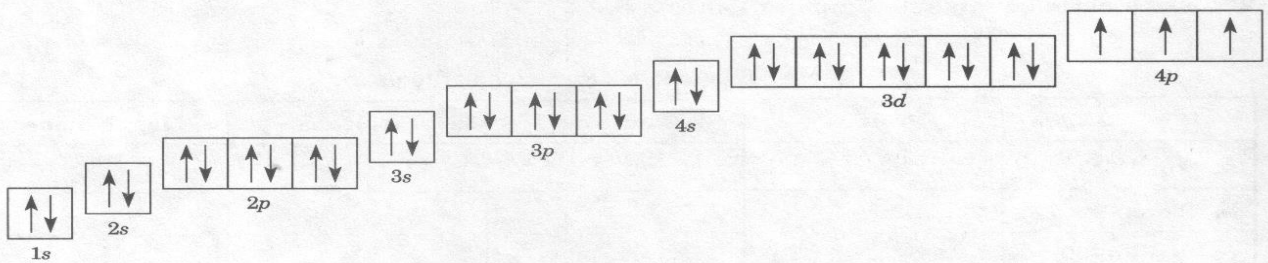
a.

a. ______________________________



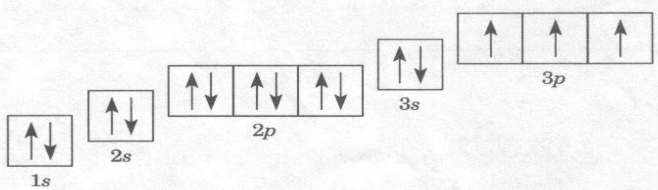
b.

b. ______________________________



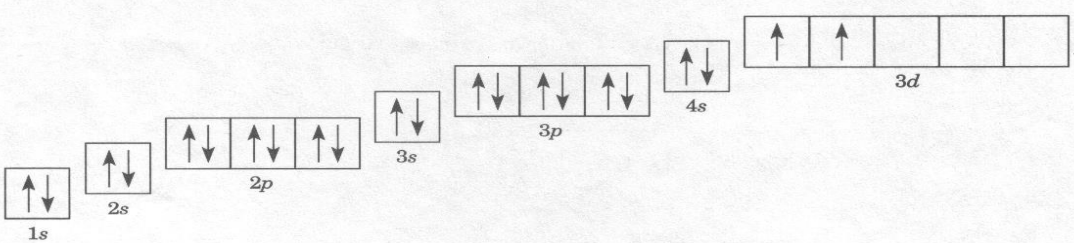
c.

c. ______________________________



d.

d. ______________________________



e.

e. ______________________________

VALENCE ELECTRONS

Name ____________________

The valence electrons are the electrons in the outermost principal energy level. They are always "s" or "s and p" electrons. Since the total number of electrons possible in s and p sublevels is eight, there can be no more than eight valence electrons.

Determine the number of valence electrons in the atoms below.

> **Example:** carbon
> Electron configuration is $1s^2$ $\boxed{2s^2\ 2p^2}$.
> Carbon has 4 valence electrons.

1. fluorine ________
2. phosphorus ________
3. calcium ________
4. nitrogen ________
5. iron ________
6. argon ________
7. potassium ________
8. helium ________
9. magnesium ________
10. sulfur ________
11. lithium ________
12. zinc ________
13. carbon ________
14. iodine ________
15. oxygen ________
16. barium ________
17. aluminum ________
18. hydrogen ________
19. xenon ________
20. copper ________

Section 5.3 Electron Configurations

In your textbook, read about ground-state electron configurations.

Use each of the terms below just once to complete the passage.

Aufbau principle	electron configuration	ground-state electron configuration	Hund's rule
lowest	Pauli exclusion principle	spins	stable

The arrangement of electrons in an atom is called the atom's **(1)** ______________________. Electrons in an atom tend to assume the arrangement that gives the atom the **(2)** ______________________ possible energy. This arrangement of electrons is the most **(3)** ______________________ arrangement and is called the atom's **(4)** ______________________.

Three rules define how electrons can be arranged in an atom's orbitals. The **(5)** ______________________ states that each electron occupies the lowest energy orbital available. The **(6)** ______________________ states that a maximum of two electrons may occupy a single atomic orbital, but only if the electrons have opposite **(7)** ______________________. **(8)** ______________________ states that single electrons with the same spin must occupy each equal-energy orbital before additional electrons with opposite spins occupy the same orbitals.

Complete the following table.

Element	Atomic Number	Orbitals					Electron Configuration
		1s	2s	$2p_x$	$2p_y$	$2p_z$	
9. Helium							$1s^2$
10.	7						
11. Neon		↑↓	↑↓	↑↓	↑↓	↑↓	

Section 5.3 ***continued***

Answer the following questions.

12. What is germanium's atomic number? How many electrons does germanium have?

____

13. What is noble-gas notation, and why is it used to write electron configurations?

____

____

____

____

14. Write the ground-state electron configuration of a germanium atom, using noble-gas notation.

____

In your textbook, read about valence electrons.

Circle the letter of the choice that best completes the statement or answers the question.

15. The electrons in an atom's outermost orbitals are called

a. electron dots. **b.** quantum electrons. **c.** valence electrons. **d.** noble-gas electrons.

16. In an electron-dot structure, the element's symbol represents the

a. nucleus of the noble gas closest to the atom in the periodic table.

b. atom's nucleus and inner-level electrons.

c. atom's valence electrons.

d. electrons of the noble gas closest to the atom in the periodic table.

17. How many valence electrons does a chlorine atom have if its electron configuration is $[Ne]3s^23p^5$?

a. 3 **b.** 21 **c.** 5 **d.** 7

18. Given boron's electron configuration of $[He]2s^22p^1$, which of the following represents its electron-dot structure?

a. •Be• **b.** •$\dot{B}$• **c.** $\ddot{B}$: **d.** $\ddot{Be}$

19. Given beryllium's electron configuration of $1s^22s^2$, which of the following represents its electron-dot structure?

a. •Be• **b.** •$\dot{B}$• **c.** $\ddot{B}$: **d.** $\ddot{Be}$

20. Which electrons are represented by the dots in an electron-dot structure?

a. valence electrons **c.** only s electrons

b. inner-level electrons **d.** both a and c