Homework Assignments:

- Increased the number of attempts to 10 in OWL homework
- Chapter 5 HW due October 11 at 11:55 pm
- Will assign Chapter 6 HW today!

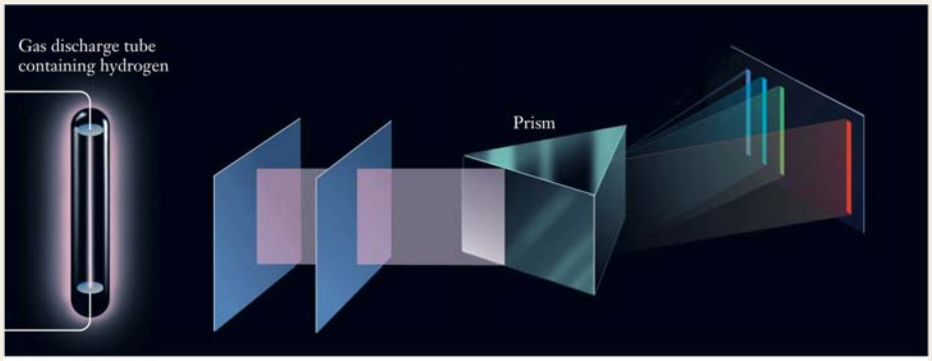
14

Atomic Spectra

- Atomic spectra: The pattern of wavelengths absorbed and emitted by an element

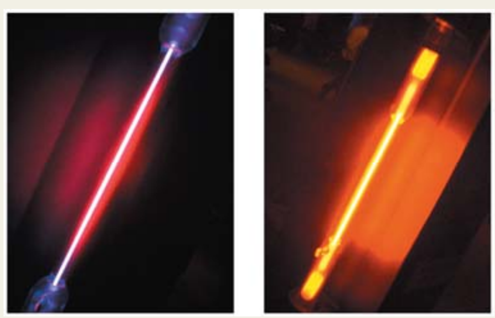
15

Atomic Spectra (continued)

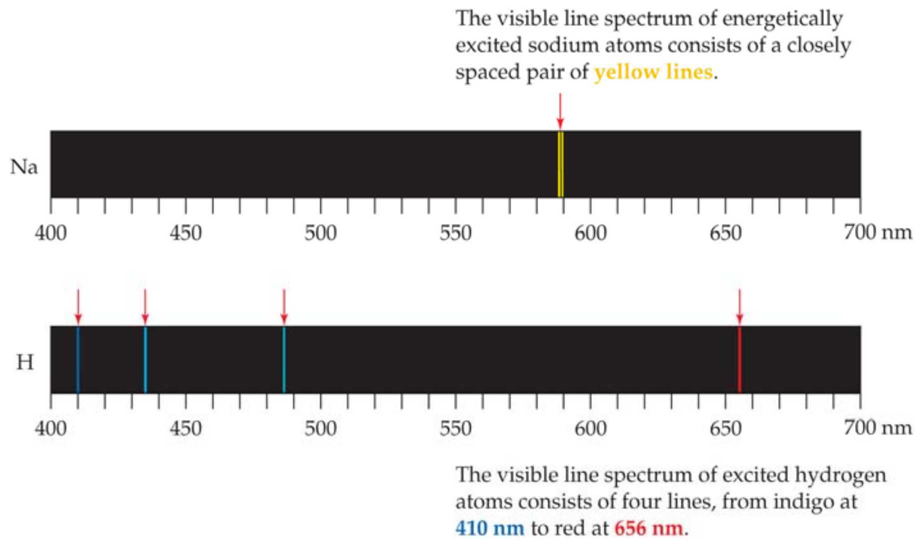


- Electrical current dissociates molecular H_2 into excited atoms, which emit light that separates into four discrete wavelengths after being passed through a prism

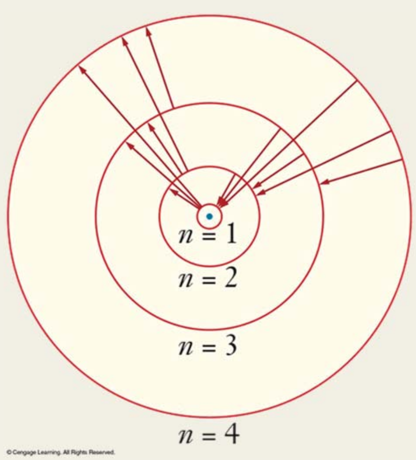
Excited hydrogen atoms give off a red light, and excited neon atoms emit orange light



Atomic line spectra



The Bohr Model of the Atom



- It can be used to explain absorption and emission
- Electrons move from low energy to higher energy orbits by absorbing energy
- Electrons move from high energy to lower energy orbits by emitting energy
- Electron energy is quantized

19

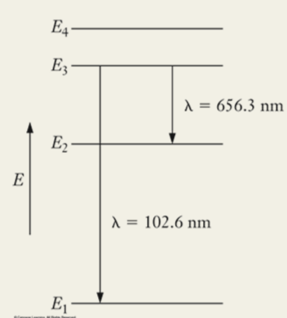
The Bohr Model of the Atom (continued)

- Excited state: When the electrons are not at the lowest possible energy state
- Ground state: When the electrons are at the lowest possible energy state
- Atoms return to ground state by emitting radiation

20

Example Problem

- When a hydrogen atom undergoes a transition from E_3 to E_1, it emits a photon with λ = 102.6 nm. Similarly, if the atom undergoes a transition from E_3 to E_2, it emits a photon with λ = 656.3 nm
  - Find the wavelength of light emitted by an atom making a transition from E_2 to E_1



Convert given λs to energies For $E_3 \longrightarrow E_1$ transition,

$$E_{3\to1} = \frac{hc}{\lambda} = \frac{(6.626 \times 10^{-34}\ \text{J s})(2.998 \times 10^{8}\ \text{m s}^{-1})}{102.6\,\text{nm}} \times \frac{10^{9}\ \text{nm}}{1\ \text{m}} = 1.936 \times 10^{-18}\ \text{J}$$

For the $E_3 \longrightarrow E_2$ transition

$$E_{3\to2} = \frac{hc}{\lambda} = \frac{(6.626 \times 10^{-34}\ \text{J s})(2.998 \times 10^{8}\ \text{m s}^{-1})}{656.3\,\text{nm}} \times \frac{10^{9}\ \text{nm}}{1\ \text{m}} = 3.027 \times 10^{-19}\ \text{J}$$

From the diagram, $E_{3\to1} = E_{3\to2} + E_{2\to1}$

So,

$$E_{2\to1} = E_{3\to1} - E_{3\to2} = 1.936 \times 10^{-18}\ \text{J} - 3.027 \times 10^{-19}\ \text{J} = 1.633 \times 10^{-18}\ \text{J}$$

Now we need to convert energy to wavelength (λ),

$$\lambda_{2\to1} = \frac{hc}{E_{2\to1}} = \frac{(6.626 \times 10^{-34}\ \text{J s})(2.998 \times 10^{8}\ \text{ms}^{-1})}{1.633\ \text{nm} \times 10^{-18}\ \text{J}} = 1.216 \times 10^{-7}\ \text{m}$$

= 121.6 nm

22

The Quantum Mechanical Model of the Atom

- Quantum mechanical model replaced the Bohr model of the atom
  - It depicts electrons as waves spread out or delocalized through a region of space called an orbital

- An orbital is characterized by three parameters called **quantum numbers**: n, l, and m_l.

23

Principal Quantum Number (*n*)

- Commonly called *shell*
- Positive integer (n = 1, 2, 3, 4, …)
- n = 1 is the first shell, n = 2 is the second shell, and so on
- Each shell has different energies

Secondary Quantum Number (*l*)

- Commonly called *subshell*
- l can have any integral value from 0 to n-1
  - If n = 1, then l = 0
  - If n = 2, then l = 0 or 1
  - If n = 3, then l = 0, 1, or 2
  - ……. and so forth

Table 6.1 Letter designations for naming orbitals

ℓ-value	0	1	2	3	4
Letter designation	*s*	*p*	*d*	*f*	*g*

Magnetic Quantum Number (m_l)

- Defines the spatial orientation of the orbital
- can have any integer value from $-l$ to $+l$
  - If $l = 0$, then $m_l = 0$
  - If $l = 1$, then $m_l = -1, 0,$ or $+1$
  - If $l = 2$, then $m_l = -2, -1, 0, +1,$ or $+2$
  - etc.

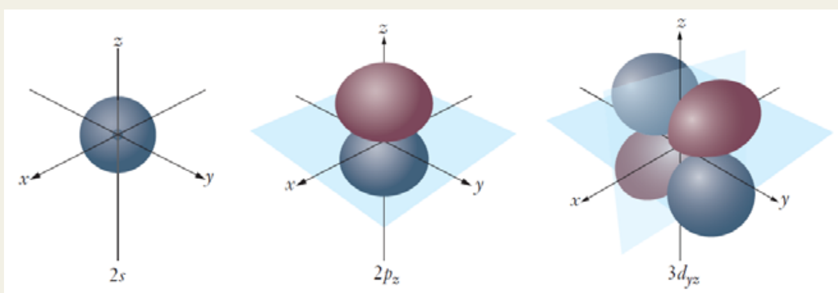
Allowed combination of quantum numbers:

Value of n	Values for ℓ (letter designation)	Values for m_ℓ	Number of Orbitals
1	0 (s)	0	1
2	0 (s)	0	1
	1 (p)	−1, 0, 1	3
3	0 (s)	0	1
	1 (p)	−1, 0, 1	3
	2 (d)	−2, −1, 0, 1, 2	5
4	0 (s)	0	1
	1 (p)	−1, 0, 1	3
	2 (d)	−2, −1, 0, 1, 2	5
	3 (f)	−3, −2, −1, 0, 1, 2, 3	7

Example Problem

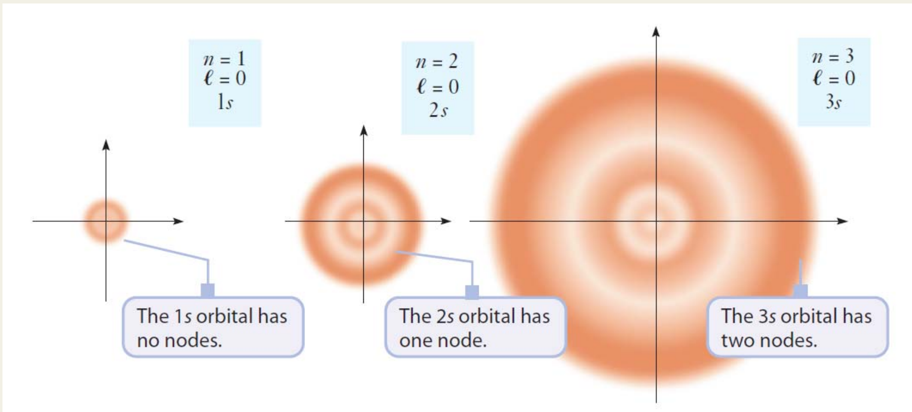
- Write all of the allowed sets of quantum numbers (*n*, *l*, and m_l) for a 3p orbital

Visualizing Orbitals



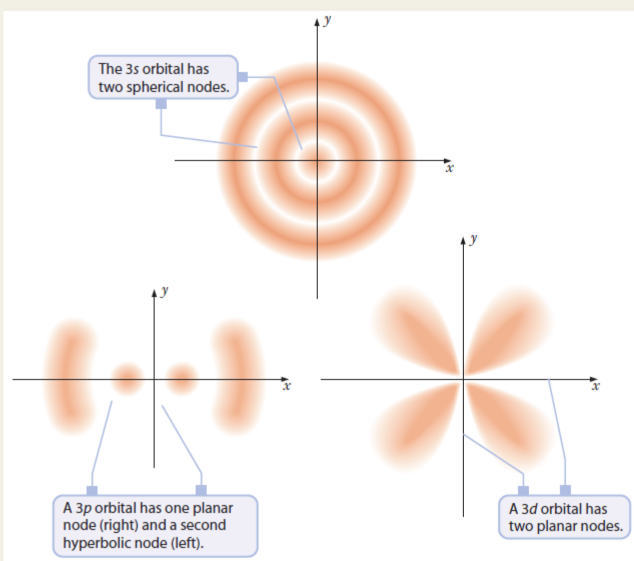
- *s* orbitals are spherical
- *p* orbitals have two lobes separated by a nodal plane
  - A nodal plane is a plane where the probability of finding an electron is zero
  - Here, it is the *xy* plane
- *d* orbitals have more complicated shapes due to the presence of two nodal planes

Visualizing Orbitals



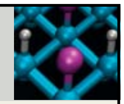
Cross-sectional views of the 1*s*, 2*s*, and 3*s* orbitals

Visualizing Orbitals



- Electron density plots for 3*s*, 3*p*, and 3*d* orbitals showing the nodes in each orbital

Spin quantum number (m_s)



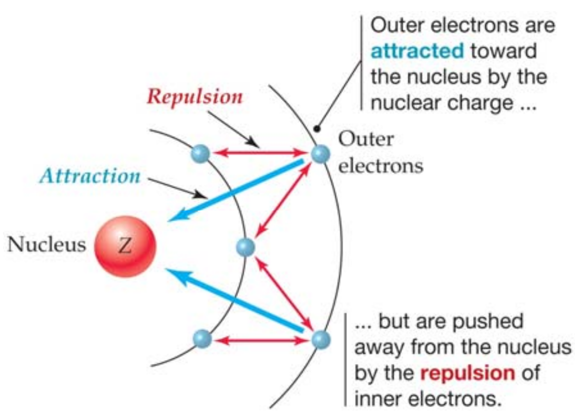
- Electrons have spin, which gives rise to a tiny magnetic field and to a **spin quantum number (m_s),** which can have +1/2 or -1/2

32

Effective Nuclear Charge (*ENC*): The nuclear charge actually felt by an electron.

- Masking of the nuclear charge is called shielding
- Shielding results in a reduced, effective nuclear charge

ENC = Actual nuclear charge (NC) – Electron shielding



Problem

In most cases, how is effective nuclear charge (ENC) related to nuclear charge (NC) for an atom?

- ENC < NC
- ENC = NC
- ENC > NC

Answer: ENC < NC

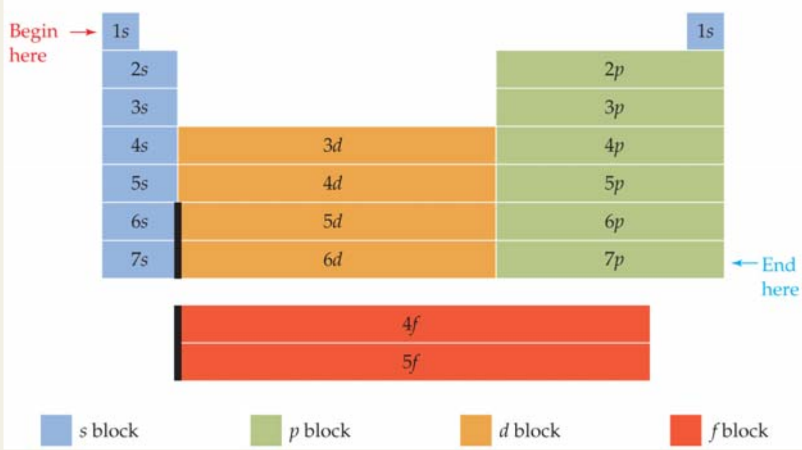
34

The Periodic Table and Electron Configurations

- The periodic table is broken into *s*, *p*, *d*, and *f* blocks
- Structure of periodic table can be used to predict the orbital filling order that leads to write electron configurations for most elements

35

The arrangement of the periodic table provides a method for remembering the order of orbital filling. Beginning at the top left and moving across successive rows, the order is 1s → 2s → 2p → 3s → 3p → 4s → 3d → 4p and so on.



Entire orbital filling order of electrons:

$1s \rightarrow 2s \rightarrow 2p \rightarrow 3s \rightarrow 3p \rightarrow 4s \rightarrow 3d \rightarrow 4p \rightarrow 5s \rightarrow 4d \rightarrow 5p \rightarrow$
$6s \rightarrow 4f \rightarrow 5d \rightarrow 6p \rightarrow 7s \rightarrow 5f \rightarrow 6d \rightarrow 7p$

36

Hund's Rule and the Aufbau Principle

- Aufbau principle - Lower energy orbital fill before higher energy orbitals
- Hund's rule states that within a subshell, electrons occupy orbitals individually and with spin paired whenever possible. One with spin up and other with spin down
- An orbital can hold two electrons only
- Electron configurations are sometimes depicted using boxes to represent orbitals
- This depiction shows paired and unpaired electrons
  - See the example for carbon below: