Chapter 5

- water molecule, $H_2O$
  
  2 H atoms (O)
  (O) O atom

- how do these atoms differ?

  # subatomic particles
  atomic weight: O - 16 amu, H - 1 amu

- why do they weigh different amounts?
- what are atoms "made of"?

\[
\begin{array}{ccc}
\text{subatomic} & \text{particles} & \\
\text{electron} & 0.00055 \text{ amu} & -1 \ \ \ \ \ \ \ \ \ \ \ \ e^- \\
\text{proton} & 1.0073 \text{ amu} & +1 \ \ (p \ or \ p^+) \\
\text{neutron} & 1.0087 \text{ amu} & 0 \ \ (n \ or \ n^+) \\
\end{array}
\]

- electrons - a stream of them
  - can be deflected by magnets
  - "voltage difference"

- casts a shadow (like light)
- can turn a paddlewheel (like a stream of particles)
- move toward anode - negative charge
Protons
- move toward cathode (positively charged)
- more than 1800x heavier than electrons

Neutrons - weigh slightly more than a proton.

So, atoms are made of protons, electrons, & neutrons.

How many in H? in O? of each kind?

Atomic number - the # of protons in each atom

(listed above each element's symbol on Periodic Table)

O - 8 protons 8 electrons
H - 1 proton 1 electron
Cl - 17 protons 17 electrons

* For a neutral atom, \( \# \) protons = \( \# \) electrons

Look @ P.T. elements are arranged by increasing atomic #.
Atomic # is pretty important to element identity. In fact,
* the # of protons (atomic #) is what makes each kind of atom unique.
For \( \text{H} \), atomic mass = 1.0079 amu

\( 1 \) proton + \( 1 \) electron = 1.0073 + 0.00055 = 1.0078 amu

pretty close.

but for \( \text{O} \), atomic mass = 15.9994 amu

8 protons + 8 electrons ≠ 15.9994 amu, not even close.

oxygen must contain neutrons. but how many?

mass number = # protons + # neutrons (counted, not measured)

note: mass ≠ atomic mass

but this number is not given on the periodic table. why?

isotope - atoms of the same element with different masses due to a different # of neutrons.

?!! how is this possible? periodic table gives us one atomic mass per element! How can there be more than one mass for the same element???

- # protons makes an atom unique (#electrons = # protons in a neutral atom)

- atomic mass is a weighted average of the different masses of naturally occurring isotopes for a particular kind of atom.
ex. the two most naturally occurring isotopes of Cl are

\[ ^{35}\text{Cl} \]  (17 protons + 18 neutrons) \ 91.84 \text{ abundance} \\
\[ ^{37}\text{Cl} \]  (17 protons + 20 neutrons) \ 8.06 \text{ abundance} \\

calculate the atomic mass of Cl.

\[
\begin{align*}
\frac{0.008}{17} (1.0073) & + (17)(0.00055) + 18 (1.0087) = 35.29 \text{amu} \\
\frac{17 (1.0073) + (17)(0.00055) + 20 (1.0087)}{2} & = 37.30 (75) \text{amu} \\
\end{align*}
\]

\[
(0.9194(35.29) + 0.0806)(37.3075) = 35.45
\]

Nucleide symbol: \[ E \]

\[ z \] element symbol
\[ A \] mass number
\[ z \] atomic number

\[ ^{35}\text{Cl} \] \[ ^{37}\text{Cl} \]

hydrogen has three isotopes that are important enough to have special names:

\[ ^{1}\text{H} \] hydrogen
\[ ^{2}\text{H} \] deuterium
\[ ^{3}\text{H} \] tritium

1 proton
1 proton
1 proton

1 electron
1 electron
1 electron

0 neutrons
1 neutron
2 neutrons

radioactive
Some elements have only one, naturally occurring isotope (e.g., F, Al) but most occur in nature as mixtures.

Another ex.

Boron weighs 10.811 amu. Masses of its 2 isotopes are

\[ ^{10}B = 10.013 \text{ amu} \quad \text{and} \quad ^{11}B = 11.009 \text{ amu} . \]

What are the % abundances?

\[ x + y = 1 \]
\[ y = 1 - x \]

\[ x(10.013) + (1-x)(11.009) = 10.811 \]

\[ 0.996x = -0.198 \]
\[ x = 0.198 \times 100 \]
\[ x = 19.8\% \]
\[ y = 80.12\% \]
H atom & O atom

now we know
- what's in it
- how much of each thing is in it.

but where is it?
how are the subatomic particles arranged?

Various theories
- proton "pudding" with electrons like raisins
  Floating around in it.

Rutherford's scattering experiments located a very small,
very dense center of mass - called nucleus

protons & neutrons are in nucleus. Electrons are floating
around nucleus (orbiting), a little like a planet
orbiting around the sun.

If this classroom were a nucleus, we'd have to drive all the
way to Austin to find the nearest electron.

Atoms are mostly empty space.
Where are the electrons?

- Not random - electrons are organized.
- Outer limits - dominating factor in their chemical behavior.

Spectroscopy - the study of the interaction of electromagnetic radiation with matter.

Electromagnetic radiation - energy that:
- a) travels through space in waves
- b) has electric & magnetic field components
- c) falls in a certain energy range.

Plan: expose matter to different kinds of energy & see what happens.
Get clues about organization of electrons.

\[
\text{wavelength (}\lambda\text{)} - \text{distance between 2 adjacent, identical points on the wave}
\]

\[
\text{Frequency (}\nu\text{)} - \# \text{ crests passing a point per given amount of time (cycles/second)}
\]

\[
\begin{align*}
\lambda & \quad \text{longer wavelength} \\
\lambda & \quad \text{lower frequency}
\end{align*}
\]

\[
\begin{align*}
\lambda & \quad \text{shorter wavelength} \\
\lambda & \quad \text{higher frequency}
\end{align*}
\]
\[ \lambda \nu = \text{speed of propagation} = c \text{ (for electromagnetic radiation)} = 3 \times 10^8 \text{ m/s} \]

\[ \nu = \frac{c}{\lambda} \]

- Fig 5.12b. - 1 Ångstrom = \(1 \times 10^{-10}\) m

light as waves
light as particles How? Why?

How? call light particle a photon (weightless particle)
- each photon has a particular amount of energy a quantum "packet"

(hugar)

(E) Energy of photon depends on frequency

\[ E_p = h \nu \]

\[ h = \text{Planck's constant} \approx 6.626 \times 10^{-34} \text{ J.s} \]

in terms of wavelength

\[ E_p = \frac{hc}{\lambda} \]

\( \lambda \uparrow E \uparrow \)

\( \lambda \uparrow E \downarrow \)

\[ E \lambda = hc \]
Why?  

**photoelectric effect**  
(Einstein)  
(Nobel Prize in Physics)

- hit metal surface with high energy light
- electrons "knocked out", as if they've been hit
- certain wavelength threshold

- smaller wavelength ≠ more electrons ejected
- brighter light source = more electrons ejected

(sugar)

Spectroscopy] → add energy & see what happens  
added light & knocked out electrons  
possibilities are endless!

Can add energy such that photons come out  
emission spectrum

zap vaporized atoms (at low pressure) w/electric current.

Figure 5.15, 5.14.

light emitted at discrete energies (certain wavelengths)  
why? because electrons are organized.

Bohr model for atom - electrons travel around nucleus  
in circular orbits

Energy is quantized.
ex. orange light has wavelength 5890 Å. Calculate $E$ for one photon of orange light.

$$E = \frac{hc}{\lambda}$$
$$E = \frac{(6.626 \times 10^{-34} \text{ J} \cdot \text{s})(3.0 \times 10^8 \text{ m/s})}{5890 \times 10^{-10} \text{ m}}$$
$$E = 3.4 \times 10^{-19} \text{ J per photon}$$
H atom (a 1e\textsuperscript{-} system)
- emission lines can be assigned to specific E transitions
- more complicated atoms (more than 1e\textsuperscript{-})
  - Bohr theory breaks down - can't explain data.

Why?
Bohr approach - classical mechanics
doesn't work for very small particles
quantum mechanics - new physics to deal with very small particles
retain from Bohr:
  - electrons are ordered (orbitals)
  - energy levels are quantized.

\textit{\textbf{wave, recall,}} light can be treated as \underline{particle} or \underline{wave}
electron can be treated as \underline{particle} or \underline{wave}

de Broglie \[ \lambda = \frac{h}{mv} \quad m = \text{mass} \quad v = \text{speed} \]
e\textsuperscript{-} @ \(1.24 \times 10\textsuperscript{7} \text{ m/s}\), \[ \lambda = 5.87 \times 10\textsuperscript{-11} \text{ m} = 0.0587 \text{ nm or } 0.587 \text{ Å} \]
green light \( \lambda = 4.86 \times 10\textsuperscript{-7} \text{ m} = 486 \text{ nm or } 0.486 \text{ Å} \)
electrons can give you a better resolution picture (smaller), \underline{better-resolution electron microscopy}. 
where are electrons?
- use quantum mechanics to find them
- treat electrons as waves, not particles

Problem
Heisenberg uncertainty principle - it is not possible to determine (simultaneously) the position & momentum of an electron (momentum = \( m \times v \))

why? measurement itself perturbs system, measurements involve electromagnetic radiation (spectroscopy) - makes electrons "hop".

instead of locating electron precisely, we can plot a map of the probability of where we will find it - call this map an atomic orbital.

Schrödinger equation - differential equation describing a 3-d standing wave, used to treat electrons as waves in quantum mechanics.
Basic ideas of quantum mechanics

1) atoms & molecules can only exist in certain energy states when state changes, must absorb (or emit) exactly the amount of required energy. Quantized. (Bohr model & photoelectric effect)

2) Emitting/absorbing radiation changes energies by the following equation
   \[ \Delta E = h \frac{\nu}{\lambda} \] (line emission spectra)

3) the allowed energy states of atoms & molecules can be described by quantum numbers.

Quantum numbers - numbers that describe the different energy levels of the electrons in a system

Use quantum numbers to

1) keep track of electrons (organized)
2) get pictures of atomic orbitals (probability maps for \( e^- \))
4. quantum numbers

1. principal quantum number, \( n \)
   main energy level (shell)
   \( n = 1, 2, \ldots, \infty \)

2. angular quantum number, \( l \)
   shape of region that e\(^{-}\) occupies (subshell)
   \( s, p, d, f \)
   \( l = 0, 1, 2, 3, \ldots (n-1) \)

3. magnetic quantum number, \( m_l \)
   specific orbital in a subshell
   directions are different but \( E \) is the same
   \( m_l = -l, \ldots, l \)

4. spin quantum number
   every orbital holds 2 electrons
   \( m_s = \pm \frac{1}{2} \)

Pauli exclusion principle - no two electrons in an atom may have identical sets of quantum numbers
ex. How many subshells are found in the shell $n=3$?

how many orbitals?

how many electrons?

$n = 3$  $l = 0, 1, 2$  $m_e = -l \ldots + l$

$s$  $p$  $d$

$n = 3$  $l = 0$  $m_e = 0$  $3s$  1

$n = 3$  $l = 1$  $m_e = -1$  $3p$  3

$n = 3$  $l = 1$  $m_e = 0$  $3p$  3

$n = 3$  $l = 1$  $m_e = +1$  $3p$  3

$n = 3$  $l = 2$  $m_e = -2$  $3d$  5

$n = 3$  $l = 2$  $m_e = -1$  $3d$  5

$n = 3$  $l = 2$  $m_e = 0$  $3d$  5

$n = 3$  $l = 2$  $m_e = 1$  $3d$  5

$n = 3$  $l = 2$  $m_e = 2$  $3d$  5

- 3 subshells
- 9 orbitals
- 18 electrons.
what do orbitals look like?

principal - main E level (size)
angular - shape
magnetic - direction

plot simplest: \( n=1, \ l=0, \ m_l=0 \) (Fig. 5-20)
- cross section is circle
- \( l=0 \) (s) is sphere-shaped
- for \( n=2,3 \) still spheres but bigger

what about other shapes?
- Fig 5-21 \( l=1 \) (p). dumbbell
  \( m_l=-1,0,1 \) direction?
- Fig 5-23 \( px, py, pz \)

\( l=2 \) (d) Fig 5-24
  \( m_l=-2,-1,0,1,2 \)

Shapes of atomic orbitals help determine shapes of molecules
Now we know where the electron is, if it's in an orbital. But how do we know whether or not a particular orbital has an electron in it?

Fill lowest energy orbitals first.

**Ground state electron configuration** - atom in its lowest energy state.

**Aufbau principle** - put electrons into orbitals from lowest energy up ("building up")

- Fill each shell first \((n)\) from lowest to highest
- Fill subshells in this order: \(s < p < d < f\).

- Atomic orbital
- \(1\) unpaired electron
- \(1\) paired electrons \((\rightarrow\text{Forbidden by Pauli exclusion principle})\)

<table>
<thead>
<tr>
<th>Atomic Number</th>
<th>Orbitals</th>
<th>Notation</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>(1)</td>
<td>(1s^1)</td>
</tr>
<tr>
<td>2</td>
<td>(1)</td>
<td>(1s^2)</td>
</tr>
</tbody>
</table>

\(n = 1\) row 1
n = 2, row 2, Periodic Table

<table>
<thead>
<tr>
<th>1s</th>
<th>2s</th>
<th>2p</th>
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</thead>
<tbody>
<tr>
<td>Li</td>
<td>??</td>
<td>?</td>
</tr>
<tr>
<td>Be</td>
<td>??</td>
<td>??</td>
</tr>
<tr>
<td>B</td>
<td>??</td>
<td>??</td>
</tr>
<tr>
<td>C</td>
<td>??</td>
<td>??</td>
</tr>
<tr>
<td>N</td>
<td>??</td>
<td>??</td>
</tr>
<tr>
<td>O</td>
<td>??</td>
<td>??</td>
</tr>
</tbody>
</table>

Hund’s rule – electrons occupy all orbitals of a subshell singly before pairing begins

<table>
<thead>
<tr>
<th>F</th>
<th>??</th>
<th>??</th>
<th>??</th>
<th>??</th>
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</thead>
<tbody>
<tr>
<td>Ne</td>
<td>??</td>
<td>??</td>
<td>??</td>
<td>??</td>
</tr>
</tbody>
</table>

Paramagnetic – atom has unpaired electrons (B, C, N, O, F)

Diamagnetic – atom has no unpaired electrons (Be, Ne)
Chapter 5 lecture notes

n = 3, row 3, Periodic Table  shorthand for filled subshells 1 & 2: \([\text{Ne}]\)

<table>
<thead>
<tr>
<th></th>
<th>3s</th>
<th>3p</th>
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</thead>
<tbody>
<tr>
<td>Na</td>
<td>([\text{Ne}])</td>
<td>?</td>
</tr>
<tr>
<td>Mg</td>
<td>([\text{Ne}])</td>
<td>??</td>
</tr>
<tr>
<td>Al</td>
<td>([\text{Ne}])</td>
<td>??</td>
</tr>
<tr>
<td>Si</td>
<td>([\text{Ne}])</td>
<td>??</td>
</tr>
<tr>
<td>Ar</td>
<td>([\text{Ne}])</td>
<td>??</td>
</tr>
</tbody>
</table>

\[ n = 4, \text{row 4, Periodic table } \text{but wait! Haven’t filled 3d yet!} \]

\[ n + 1 \text{ filling rules } – \]

\[ 4s \text{ goes in before 3d} \]
\[ 5s \text{ goes in before 4d} \]
\[ 6s \text{ goes in before 5d} \]

<table>
<thead>
<tr>
<th></th>
<th>3d</th>
<th>4s</th>
<th>4p</th>
</tr>
</thead>
<tbody>
<tr>
<td>K</td>
<td>([\text{Ar}])</td>
<td>==</td>
<td>==</td>
</tr>
<tr>
<td>Ca</td>
<td>([\text{Ar}])</td>
<td>==</td>
<td>==</td>
</tr>
<tr>
<td>Sc</td>
<td>([\text{Ar}])</td>
<td>?</td>
<td>==</td>
</tr>
<tr>
<td>Ti</td>
<td>([\text{Ar}])</td>
<td>?</td>
<td>?</td>
</tr>
<tr>
<td>V</td>
<td>([\text{Ar}])</td>
<td>?</td>
<td>?</td>
</tr>
<tr>
<td>Cr</td>
<td>([\text{Ar}])</td>
<td>?</td>
<td>?</td>
</tr>
</tbody>
</table>

\[ \text{Exception – half-filled & completely filled subshells are more stable (sometimes)} \]

<table>
<thead>
<tr>
<th></th>
<th>3d</th>
<th>4s</th>
<th>4p</th>
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<tbody>
<tr>
<td>Mn</td>
<td>([\text{Ar}])</td>
<td>==</td>
<td>==</td>
</tr>
<tr>
<td>Cu</td>
<td>([\text{Ar}])</td>
<td>==</td>
<td>==</td>
</tr>
<tr>
<td>Zn</td>
<td>([\text{Ar}])</td>
<td>==</td>
<td>==</td>
</tr>
<tr>
<td>Ga</td>
<td>([\text{Ar}])</td>
<td>==</td>
<td>==</td>
</tr>
<tr>
<td>Ge</td>
<td>([\text{Ar}])</td>
<td>==</td>
<td>==</td>
</tr>
</tbody>
</table>

\[ \text{exceptions: Cr, Mo; Cu, Ag, Au.} \]
Chapter 5 lecture notes

**General guide to filling: Fig 5-29.**

<table>
<thead>
<tr>
<th>8s</th>
<th>7s</th>
<th>7p</th>
</tr>
</thead>
<tbody>
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<td>6p</td>
<td>6d</td>
</tr>
<tr>
<td>5s</td>
<td>5p</td>
<td>5d</td>
</tr>
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<td>4s</td>
<td>4p</td>
<td>4d</td>
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<tr>
<td>3s</td>
<td>3p</td>
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<td>2p</td>
<td></td>
</tr>
<tr>
<td>1s</td>
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</table>

<table>
<thead>
<tr>
<th>4f</th>
<th>5d</th>
<th>6s</th>
<th>6p</th>
</tr>
</thead>
<tbody>
<tr>
<td>Ta</td>
<td>[Xe]</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Ta&lt;sup&gt;2+&lt;/sup&gt;</td>
<td>[Xe]</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

[Table with elements and electron configurations]
Understanding oxidation numbers:

<table>
<thead>
<tr>
<th>3s</th>
<th>3p</th>
</tr>
</thead>
<tbody>
<tr>
<td>Na</td>
<td>[Ne]</td>
</tr>
<tr>
<td>Al</td>
<td>[Ne]</td>
</tr>
<tr>
<td>Cl</td>
<td>[Ne]</td>
</tr>
</tbody>
</table>

4d 5s 5p

Zr [Kr] = = = = = = = = = =

Isoelectronic – two (or more) species having the same number of electrons

Assigning quantum numbers

Na: $n = 3, l = 0, m_l = 0, m_s = +1/2$
Al: $n = 3, l = 0, m_l = 0, m_s = +1/2, - 1/2$
    $n = 3, l = 1, m_l = -1, m_s = +1/2$
Zr: $n = 5, l = 0, m_l = 0, m_s = +1/2, - 1/2$
    $n = 4, l = 2, m_l = -2, m_s = +1/2$
    $n = 4, l = 2, m_l = -1, m_s = +1/2$