HOW THE ATOM CAME TOGETHER
A Brief History of Atomic Theory

Lesson #1 A Brief History of the Atom
Atomic Theory Timeline

The atomic model has changed over time.

For over two centuries, scientists have created different models of the atom.

As scientists have learned more and more about atoms, the atomic model has changed.

Atomic Theory Timeline

Dalton  Thomson  Rutherford  Bohr  Chadwick  Modern
But First, Democritus!

Democritus was a Greek philosopher (470-380 B.C.) who is the father of modern atomic thought.

He proposed that matter could NOT be divided into smaller pieces forever.

He claimed that matter was made of small, hard particles that he called “atomos”.

John Dalton - 1808

John Dalton created the very first atomic theory.

Dalton was an English school teacher who performed many experiments on atoms.

Dalton viewed atoms as tiny, solid balls.

His atomic theory had 4 statements…
Dalton’s Theory

1. Atoms are tiny, invisible particles.
2. Atoms of one element are all the same.
3. Atoms of different elements are different.

J.J. Thomson (1897)

J.J. Thomson discovered electrons.

He was the first scientist to show that the atom was made of even smaller things.

He also proposed the existence of a (+) particle…

His atomic model was known as the “raisin bun model”…
Thomson’s Model

Atoms are made mostly out of (+) charged material, like dough in a bun.

The (-) charged electrons are found inside the (+) dough.

Ernest Rutherford (1911)

Rutherford discovered protons and the nucleus.

He showed that atoms have (+) particles in the center, and are mostly empty space.

He called these (+) particles protons.

He called the center of atoms the nucleus.
Rutherford’s Experiment

Radioactive material emits beam of (+) alpha particles

Gold foil

Most particles went right through!

Strangely, some particles are deflected

Rutherford’s Experiment

Gold Nucleus

Most $\alpha$ particles went through the gold. The atom is mostly empty space.
Rutherford’s Experiment

The atom had a very dense (+) center. Rutherford called it the nucleus.

Niels Bohr (1913)

Niels Bohr improved on Rutherford’s model.

He proposed that electrons move around the nucleus in specific layers, or shells.

Every atom has a specific number of electron shells.
James Chadwick (1932)

Chadwick discovered neutrons.

Working with Rutherford, he discovered particles with no charge.

He called these particles neutrons.

Neutrons are also found in the nucleus.

The Modern Model (1932-)

Work done since 1920 has changed the model.

The new atomic model has electrons moving around the nucleus in a cloud.

It is impossible to know where an electron is at any given time.
The Current Atomic Model

Atomic Theory Timeline

Dalton  Thomson  Rutherford  Bohr  Chadwick  Modern
What particles are atoms made of?

For some time, people thought that atoms were the smallest particles and could not be broken into anything smaller.

Scientists now know that atoms are actually made from even smaller particles. There are three types:

- proton
- neutron
- electron

How are these particles arranged inside the atom?
**How did our understanding change?**

**J.J Thomson** discovered **electrons**, and proposed the existence of a (+) particle.

It wasn’t until **Rutherford**’s famous gold foil experiment that the + **proton** was discovered, and atoms were thought to me mostly empty space. He named the **centre of atoms** the **nucleus**.

**Bohr** improved on this model proposing that electrons move around the nucleus in specific layers called **shells**.

It was James **Chadwick** who discovered particles with **no charge**, which he named **neutrons**.

---

**What is the structure of an atom?**

Protons, neutrons and electrons are not evenly distributed in an atom.

The protons and neutrons exist in a dense core at the centre of the atom. This is called the **nucleus**.

The electrons are spread out around the edge of the atom. They orbit the nucleus in layers called **shells**.
There are two properties of protons, neutrons and electrons that are especially important:

- mass
- electrical charge.

<table>
<thead>
<tr>
<th>Particle</th>
<th>Mass</th>
<th>Charge</th>
</tr>
</thead>
<tbody>
<tr>
<td>proton</td>
<td>1</td>
<td>+1</td>
</tr>
<tr>
<td>neutron</td>
<td>1</td>
<td>0</td>
</tr>
<tr>
<td>electron</td>
<td>almost 0</td>
<td>-1</td>
</tr>
</tbody>
</table>

The atoms of an element contain equal numbers of protons and electrons and so have no overall charge.
How many electrons?

Atoms have no overall electrical charge and are neutral. This means atoms must have an equal number of positive protons and negative electrons.

The number of electrons is therefore the same as the atomic number.

<table>
<thead>
<tr>
<th>Atoms</th>
<th>Protons</th>
<th>Neutrons</th>
<th>Electrons</th>
</tr>
</thead>
<tbody>
<tr>
<td>helium</td>
<td>2</td>
<td>2</td>
<td>2</td>
</tr>
<tr>
<td>copper</td>
<td>29</td>
<td>35</td>
<td>29</td>
</tr>
<tr>
<td>iodine</td>
<td>53</td>
<td>74</td>
<td>53</td>
</tr>
</tbody>
</table>

Atomic number is the number of protons rather than the number of electrons, because atoms can lose or gain electrons but do not normally lose or gain protons.

Atomic Number (Z)

The number of protons in an atom is known as the atomic number or proton number.

- always the same for a particular element.
- The number of protons identifies the element!
- is also equal to the positive charge of the nucleus (aka the ________________).

Example:

If an atom has \( Z = 12 \), then it MUST be an atom of ________________
If an ion has \( Z = 41 \), then it MUST be an ion of ________________
If the nuclear charge of a species is +24, then it MUST be an atom or ion of ________________

The overall charge on an atom is zero because
- the number of __________ = number of __________

The charge on any ion = number of e\(^-\) __________ ( __________ )
or ________________ ( __________ ).

It is the smaller of the two numbers shown in most periodic tables. (usually on top...depends where you're looking)
Mass Number (A)

mass number = number of protons + number of neutrons

Electrons have a mass of almost zero, which means that the mass of each atom results almost entirely from the number of protons and neutrons in the nucleus.

- Does not appear in the periodic table! (not in this exact form)
- Can be expressed in number of ways:
  Carbon-12 or _____ or _____
- Does not uniquely identify the element!
  e.g. \( ^3\text{H} : __ \text{p}, __ \text{n} \) , \( ^3\text{He} : __ \text{p}, __ \text{n} \)

The larger of the two numbers shown in most periodic tables, which you are probably familiar with is mass….actually shows the relative _____________.

What’s the mass number?

mass number = number of protons + number of neutrons

What is the mass number of these atoms?

<table>
<thead>
<tr>
<th>Atoms</th>
<th>Protons</th>
<th>Neutrons</th>
<th>Mass number</th>
</tr>
</thead>
<tbody>
<tr>
<td>helium</td>
<td>2</td>
<td>2</td>
<td>4</td>
</tr>
<tr>
<td>copper</td>
<td>29</td>
<td>35</td>
<td>64</td>
</tr>
<tr>
<td>cobalt</td>
<td>27</td>
<td>32</td>
<td>59</td>
</tr>
<tr>
<td>iodine</td>
<td>53</td>
<td>74</td>
<td>127</td>
</tr>
<tr>
<td>germanium</td>
<td>32</td>
<td>41</td>
<td>73</td>
</tr>
</tbody>
</table>
**How many neutrons?**

Number of neutrons = mass number - number of protons

Number of neutrons = mass number - atomic number

How many neutrons are there in these atoms?

<table>
<thead>
<tr>
<th>Atoms</th>
<th>Mass number</th>
<th>Atomic number</th>
<th>Neutrons</th>
</tr>
</thead>
<tbody>
<tr>
<td>helium</td>
<td>4</td>
<td>2</td>
<td>2</td>
</tr>
<tr>
<td>fluorine</td>
<td>19</td>
<td>9</td>
<td>10</td>
</tr>
<tr>
<td>strontium</td>
<td>88</td>
<td>38</td>
<td>50</td>
</tr>
<tr>
<td>zirconium</td>
<td>91</td>
<td>40</td>
<td>51</td>
</tr>
<tr>
<td>uranium</td>
<td>238</td>
<td>92</td>
<td>146</td>
</tr>
</tbody>
</table>

**What are isotopes?**

Isotopes are atoms of the same element that contain different numbers of neutrons.

The reactivity of different isotopes of an element is identical because they have the same number of electrons.

The different masses of the atoms means that physical properties of isotopes are slightly different.
Isotopes

Only a few elements (e.g. phosphorus) are monoisotopic (only have one naturally occurring isotope).

Most elements (e.g. sulfur) have two or more isotopes.

Question: Why doesn’t mass number appear on the periodic table?

Answer: Because mass numbers are specific to particular isotopes and most elements are actually a blend of two or more isotopes.

e.g. Indium has two isotopes: Indium-113 and Indium-115.

Indium is 4.29% $^{113}\text{In}$ which has an isotopic mass of 112.904061 u and 95.71% $^{115}\text{In}$ which has an isotopic mass of 114.903878 u.

The relative atomic masses in the periodic table are the weighted averages of the isotopic masses of each element.

Isotopes of chlorine

About 75% of naturally-occurring chlorine is chlorine-35 ($^{35}\text{Cl}$) and 25% is chlorine-37 ($^{37}\text{Cl}$).
Isotopes of carbon

There is also more than one isotope of carbon:

<table>
<thead>
<tr>
<th>Isotope</th>
<th>Protons</th>
<th>Neutrons</th>
</tr>
</thead>
<tbody>
<tr>
<td>$^{12}\text{C}$</td>
<td>6</td>
<td>6</td>
</tr>
<tr>
<td>$^{13}\text{C}$</td>
<td>6</td>
<td>7</td>
</tr>
<tr>
<td>$^{14}\text{C}$</td>
<td>6</td>
<td>8</td>
</tr>
</tbody>
</table>

All isotopes of carbon have 6 protons and so have 6 electrons.

Because chemical reactivity depends on the number of electrons the reactivity of the isotopes of carbon is identical.

‘Weighing’ atoms

Mass spectrometry is an accurate instrumental technique used to determine the relative isotopic mass (mass of each individual isotope relative to carbon-12) and the relative abundance for each isotope. From this, the relative atomic mass of the element can be calculated.

Some uses of mass spectrometry include:

- carbon-14 dating
- detecting illegal drugs
- forensic science
- space exploration.
Mass spectrometry

How does a mass spectrometer work?

A mass spectrometer is used to determine the relative isotopic mass and the relative abundance for each isotope in a sample.

Click "play" to find out how it works.

Mass spectra of monatomic elements

The information recorded during the process of mass spectrometry is displayed as a mass spectrum.

Click "play" to find out more.
What is relative atomic mass?

The relative atomic mass \((A_r)\) of an element is the mass of one of its atoms relative to \(\frac{1}{12}\) the mass of one atom of carbon-12.

\[
relative \ atomic \ mass \ (A_r) = \frac{average \ mass \ of \ an \ atom \times 12}{mass \ of \ one \ atom \ of \ carbon-12}
\]

Most elements have more than one isotope. The \(A_r\) of the element is the average mass of the isotopes taking into account the abundance of each isotope. This is why the \(A_r\) of an element is frequently not a whole number.
Using mass spectra to calculate $A_r$

The mass spectrum of an element indicates the mass and abundance of each isotope present. For example, the mass spectrum of boron indicates two isotopes are present:

How can this be used to calculate the $A_r$ of boron?

Calculating $A_r$

Most elements have more than one isotope. The relative atomic mass of the element is the average mass of the isotopes taking into account the abundance of each isotope.

Example: what is the $A_r$ of boron?

In a sample of boron, 20% of the atoms are $^{10}$Br and 80% are $^{11}$Br.

If there are 100 atoms, then 20 atoms would be $^{10}$Br and 80 atoms would be $^{11}$Br.

The relative atomic mass is calculated as follows:

$$A_r \text{ of Br} = \text{______________}$$
Calculating $A_r$ of magnesium

In a sample of magnesium, 79.0% of the magnesium atoms are $^{24}\text{Mg}$, 10.0% are $^{25}\text{Mg}$ and 11.0% are $^{26}\text{Mg}$.

Example: What is the $A_r$ of magnesium?

1. Calculate mass $\times$ abundance of each isotope
   $\begin{align*}
   24 \times 79.0 \\
   25 \times 10.0 \\
   26 \times 11.0
   \end{align*}$

2. Add these values, and divide by 100
   $(1896 + 250 + 286) / 100$

$A_r$ of Mg = 24.3

Atomic Mass vs Mass Number

The atomic mass (or atomic weight) of each element is the weighted* average of the masses of its isotopes where the weighting depends on the abundance of each isotope in nature. Roughly speaking, the atomic mass is closest to isotopic mass of the most abundant isotope. The units are unified atomic mass units, $u$.

* Note: Mass number $\neq$ atomic mass. The textbook is too simplistic and so the notes above are what you should study.

Example 1: Magnesium has 3 naturally occurring isotopes which are listed:

<table>
<thead>
<tr>
<th>Isotope</th>
<th>Isotopic mass (u)</th>
<th>% Abundance</th>
</tr>
</thead>
<tbody>
<tr>
<td>Mg-24</td>
<td>23.985042</td>
<td>78.99</td>
</tr>
<tr>
<td>Mg-25</td>
<td>24.985837</td>
<td>10.00</td>
</tr>
<tr>
<td>Mg-26</td>
<td>25.982593</td>
<td>11.01</td>
</tr>
</tbody>
</table>
Example 2: Naturally occurring samples of carbon are 98.93% carbon-12 (isotopic mass = 12.0000 u) and 1.07% carbon-13 (isotopic mass = 13.0034 u).

a) Calculate the expected atomic mass of carbon.

b) Calculate the molar mass of carbon.

Working out relative atomic mass

Question: 1/5

Sulfur has two main isotopes in the following abundances:

$^{32}\text{S} = 96\%$ and $^{34}\text{S} = 4\%$. What is the $A_r$ of sulfur to 2dp?

Options:
- 32.08
- 32.16
- 32.24
- 32.32
Assignment #1: page 146/147 Exercises # 13-17, 19, 20, 22, 23 a-d, 25
Complete ALL assignments on a separate piece of paper and attach to your booklet when handing in at the end of the unit. Be sure to clearly number each assignment with a heading.

Lesson #3
The Electronic Structure of Atoms
Rutherford’s Model of the Atom

Recall that, in Rutherford’s model, the positively charged protons sat in the nucleus while the negatively charged electrons moved around it.
While it represented a major advance, the model could not be correct.

Here’s why:

- Opposite charges attract. So the positively-charged nucleus is very attractive to the orbiting electrons.
- Particles that move in circular paths are accelerating (otherwise, their path would be straight).
- It seemed that the electrons had to be accelerating, and thus losing energy continuously as radiation.

Waves behaving like particles? Well hit me with a Planck!

A serious challenge to Rutherford’s atomic model arose almost immediately.

By the end of the 1800s the physics available stated that accelerating charges should radiate (lose) energy.

This meant that atoms should collapse in a fraction of a second as their electrons lost energy and spiralled around the nucleus.

Rutherford’s model could not explain why the electrons didn’t lose energy and spiral into the nucleus (much like any satellite that loses gravitational energy and crashes back to Earth).
So how did we come to this, Bohr model?

The model of the atom states that a nucleus is surrounded by shells of electrons. Each shell holds a different maximum number of electrons:

- 1\textsuperscript{st} shell = 2 electrons
- 2\textsuperscript{nd} shell = 8 electrons
- 3\textsuperscript{rd} shell = 8 electrons.

At the Chemistry 11 level, this model is slightly different. Instead of electrons being arranged in shells that are a different distance from the nucleus, they are arranged in energy levels.

Physics aids The Bohr model of the atom

In 1900, Max Planck (right) developed his ‘Quantum theory’, which states that energy could be shown to behave like particles in fixed amounts he called quanta.

In 1913, Niels Bohr (left) applied Plank’s theory to electrons, and improved upon Rutherford’s model. He proposed that electrons could only exist in fixed energy levels.

The main energy levels are called principal energy levels and are given a number called the principal quantum number (n) with the lowest in energy being 1.
The Bohr Model

Each electron has a fixed energy = an energy level.

Electrons can jump from one energy level to another.

Electrons can not be or exist between energy levels.

A quantum of energy is the amount of energy needed to move an electron from one energy level to another energy level.

Understanding Bhor's Experiments

In 1913, Niels Bohr proposed a model that explained why the electrons stay in orbit! To understand the model, however, we first need to get some things straight about electromagnetic energy.

Visible light is a form of electromagnetic radiation (EMR) and all EMR is made up of photons that travel at the speed of light, c, where c = 3.00 x 10^8 m/s, or the speed of sound, 3.00 x 10^2 m/s.
Understanding Bhor’s Experiments

Solids, liquids and gases when heated under high pressure release continuous spectra. These samples emit light that contain all colours (no gaps).

Elemental gases when excited at low pressure (low density) release discontinuous spectra. These samples emit light that contain only certain coloured bands (separated by gaps).

The discontinuous pattern of light bands came to be known as a **bright line emission spectrum** or simply an emission spectrum.

Example

Determine the wavelength of sound waves with a frequency of 556 Hz.
Bhor’s experiments…

Bhor knew that when high voltage was applied across the electrodes of a sealed glass tube containing a gas such as hydrogen, the gas was heated and emitted light…he looked at this light through a spectroscope.

He saw that the spectroscope separated the light into its component wavelengths, and for hydrogen he saw a series of coloured lines against a black background.

Bhor applied quantum principles to explain the bright-line spectrum he saw for hydrogen.

Bhor’s experiments…

Bohr said that electrons travelled in specific paths called orbits. Unlike satellites orbiting the Earth, however, an electron can only change its “altitude” by gaining or losing a specific quantum (packet) of energy.

- When an electron absorbs a quantum of energy ( ) it ____________________________________________________________________________
- When an electron emits a quantum of energy ( ) it ____________________________________________________________________________
- The amount of energy must be (at least) some required multiple of _____ or a jump cannot take place.
- During a transition, the movement is instant:
  - electrons are __________ to be between __________
Model of how e+ “jump” Energy Levels

To move from one level to another, the electron must gain or lose the right amount of energy.

The required amount of energy is known as a quantum.

Here’s the idea:

Quantum Theory rescues the Nuclear Model

To move from one level to another, the electron must gain or lose the right amount of energy.

The higher the energy level, the farther it is from the nucleus.

- Gain energy to move to higher energy levels (away from nucleus)
- Lose energy to move to lower energy levels (closer to nucleus)

The degree to which they move from level to level determines the frequency of light they emit.
Bhor proposed...

The amount of energy required to go from one energy level to another is the *not same for the electrons*.

**Higher energy levels are closer together.** This means it *takes less energy* to change levels in the higher energy levels.

Once in a higher energy orbit, any electron could then return to a lower energy orbit by emitting a specific amount of energy corresponding to the energy difference.

If the frequency of that emitted energy corresponding to any part of the visible spectrum, then a bright line of that specific colour would be seen.

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An Explanation of Atomic Spectra

- The three groups of lines in the hydrogen spectrum correspond to the transition of electrons from higher energy levels to lower energy levels.
Emission Spectra

- Each transition corresponds to a certain amount of energy, known as a quantum.
- The emission spectrum for any given element is the collection of all light-emitting quantum transitions as seen through a prism or diffraction grating.

The emission spectrum of hydrogen appears below:

![Emission Spectrum of Hydrogen](image)

**Example**

Calculate the quantum of energy that must be absorbed for an electron in the hydrogen atom to jump from the 2nd energy level to the 3rd energy level (the red band seen in its emission spectrum)

\[
E = h\nu
\]

\(h\) (Planck's Constant): 
\(\nu\) (Frequency):
Bohr’s model of the hydrogen atom was successful in explaining the mystery of bright line spectra.

His calculations and predictions worked for hydrogen and he even calculated the radius of the orbit for hydrogen’s electron in its ground state.

**BUT his model failed to explain the energies absorbed and emitted by atoms with more than one electron.**

Bohr had improved the Rutherford model by incorporating quantum rules. His model explained why atoms were stable and it successfully predicted the emission spectrum for Hydrogen. Bohr’s model was ultimately deficient, however, and was replaced by the quantum mechanical model.

This model successfully predicted the emission spectrum for all the elements and - nearly 100 years later - is still the best model available.

The “birth” of quantum mechanics caused a lot of trouble, however, because accepting it meant letting go of our classical assumptions about the universe.

In the Bohr model, electrons behaved as particles in orbits around the nucleus.

In the quantum mechanical model, the electrons only predictable as waves smeared out in regions of space known as quantum orbitals or simply orbitals.
If an excited electron emits energy and drops to \( n = 2 \) from a higher energy orbit, the wavelength of the emitted energy corresponds to a particular colour of visible light. If an electron drops from \( n = 3 \) to \( n = 2 \), the energy difference between the two orbits (and therefore the energy emitted) corresponds to that of red light. Hence the red line appears in the emission spectrum. The blue-green line results from an electron transition from \( n = 4 \) to \( n = 2 \), the blue line from an electron transition from \( n = 5 \) to \( n = 2 \), and the violet line from an electron transition from \( n = 6 \) to \( n = 2 \).

This series of four bright lines in the visible spectrum is called the Balmer series, named after the Swiss schoolteacher who first derived a mathematical relationship between the lines in hydrogen’s visible emission spectrum.

**Did you know that an element can be identified by its emission spectra?**

When atoms absorb energy, electrons move into higher energy levels. These electrons then lose energy by emitting light when they return to lower energy levels.
No two elements have the same pattern of coloured bands in their emission spectra and so the emission spectrum for each element acts as its fingerprint.

Homework

Quantum Worksheet #1-10.
Lesson #4 & 5
The Quantum Mechanical Model & Electronic Structure of The Atom

Electron Arrangement
Models of atoms

Previous models of the atom state that a nucleus is surrounded by shells of electrons. Each shell holds a different maximum number of electrons:

- 1st shell = 2 electrons
- 2nd shell = 8 electrons
- 3rd shell = 8 electrons.

At the Chemistry 11 level, this model is slightly different. Instead of electrons being arranged in shells that are at a different distance from the nucleus, they are arranged in energy levels, sub-levels and orbitals.
The Bohr model of the atom

In 1900, Max Planck (right) developed his ‘Quantum theory’, which states that energy exists in fixed amounts called quanta.

In 1913, Niels Bohr (left) applied Planck’s theory to electrons. He proposed that electrons could only exist in fixed energy levels.

The main energy levels are called principal energy levels and are given a number called the principal quantum number (n) with the lowest in energy being 1.

What is ionization energy?

Ionization is a process in which atoms lose or gain electrons and become ions.

The first ionization (I₁) energy of an element is the energy required to remove one electron from a gaseous atom:

\[ \text{M}(g) \rightarrow \text{M}^+(g) + \text{e}^-(g) \]

The second ionization (I₂) energy involves the removal of a second electron:

\[ \text{M}^+(g) \rightarrow \text{M}^{2+}(g) + \text{e}^-(g) \]

Looking at trends in ionization energies can reveal useful evidence for the arrangement of electrons in atoms and ions.
Ionization energy definitions

Match the equation to the correct description

- $M^+ (g) \rightarrow M^{2+} (g) + e^- (g)$  
  second ionization energy
- $M^{3+} (g) \rightarrow M^{4+} (g) + e^- (g)$  
  third ionization energy
- $M(g) \rightarrow M^{+} (g) + e^- (g)$  
  fourth ionization energy
- $M^{2+} (g) \rightarrow M^{3+} (g) + e^- (g)$  
  first ionization energy

Evidence for Principal Energy Levels

Plotting the successive ionization energies of magnesium clearly shows the existence of different energy levels, and the number of electrons at each level.

Successive ionization energies increase as more electrons are removed.

Large jumps in the ionization energy reveal where electrons are being removed from the next principal energy level, such as between the 2nd and 3rd, and 10th and 11th ionization energies for magnesium.
More evidence for energy levels

The first ionization energies of group 2 elements also show evidence for the existence of different principal energy levels. Even though the nuclear charge increases down the group, the first ionization energy decreases.

This means electrons are being removed from successively higher energy levels, which lie further from the nucleus and are less attracted to the nucleus.

Trends in first ionization energies

First ionization energies of the first 54 elements

- Atomic number
- First ionization energy (kJ mol⁻¹)

<table>
<thead>
<tr>
<th>Atomic Number</th>
<th>First Ionization Energy (kJ mol⁻¹)</th>
</tr>
</thead>
<tbody>
<tr>
<td>2</td>
<td></td>
</tr>
<tr>
<td>10</td>
<td></td>
</tr>
<tr>
<td>18</td>
<td></td>
</tr>
<tr>
<td>36</td>
<td></td>
</tr>
<tr>
<td>54</td>
<td></td>
</tr>
</tbody>
</table>
Energy levels

What are the missing words about energy levels?

1. Evidence for the existence of different energy levels comes from studying trends in the **A** of elements.

2. The principal energy levels are labeled with numbers called principal **B** numbers, with level one being the **C** in energy.

3. The principal energy levels are the same as the **D**, which are sometimes used in

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AS Chemistry

Electron Arrangement

Energy levels

Energy sub-levels

Electron configuration

Orbitals and spin

Summary activities
Evidence for Sub-Levels

The first ionization energies for the elements in period 3 show a general increase. However, aluminium’s value is below that of magnesium. This suggests that the third principal energy level is not one single energy level.

All principal energy levels contain one or more sub-levels, with different but exact energy values.

The sub-levels

There are four sub-levels, labelled in order of increasing energy: s, p, d and f. Each holds a different number of electrons.

<table>
<thead>
<tr>
<th>sub-level</th>
<th>max no. electrons</th>
</tr>
</thead>
<tbody>
<tr>
<td>s</td>
<td>2</td>
</tr>
<tr>
<td>p</td>
<td>6</td>
</tr>
<tr>
<td>d</td>
<td>10</td>
</tr>
<tr>
<td>f</td>
<td>14</td>
</tr>
</tbody>
</table>

Each principal energy level contains a different number of sub-levels.

<table>
<thead>
<tr>
<th>principal energy level, n</th>
<th>sub-levels</th>
<th>max no. electrons</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>1s</td>
<td>2</td>
</tr>
<tr>
<td>2</td>
<td>2s, 2p</td>
<td>8</td>
</tr>
<tr>
<td>3</td>
<td>3s, 3p, 3d</td>
<td>18</td>
</tr>
<tr>
<td>4</td>
<td>4s, 4p, 4d, 4f</td>
<td>32</td>
</tr>
</tbody>
</table>
Levels and sub-levels

Principal energy levels and sub-levels

What is the relationship between electron energy levels and sub-levels?

Click "play" to find out.

Shapes of Atomic Orbitals

- Different atomic orbitals are denoted by letters.
- The s orbitals are spherical, and p orbitals are dumbbell-shaped.

- Four of the five d orbitals have the same shape but different orientations in space.
Atomic Orbitals

• The numbers and kinds of atomic orbitals depend on the energy sublevel.

<table>
<thead>
<tr>
<th>Energy Level, n</th>
<th># of sublevels</th>
<th>Letter of sublevels</th>
<th># of orbitals per sublevel</th>
<th># of electrons in each orbital</th>
<th>Total electrons in energy level</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>1</td>
<td>s</td>
<td>1</td>
<td>2</td>
<td>2</td>
</tr>
<tr>
<td>2</td>
<td>2</td>
<td>s, p</td>
<td>1</td>
<td>2</td>
<td>8</td>
</tr>
<tr>
<td>3</td>
<td>3</td>
<td>s, p, d</td>
<td>1, 3</td>
<td>2</td>
<td>18</td>
</tr>
<tr>
<td>4</td>
<td>4</td>
<td>s, p, d, f</td>
<td>1, 3, 5</td>
<td>2</td>
<td>32</td>
</tr>
</tbody>
</table>
Blocks of the periodic table

What are s, p, d and f blocks?
Click a shaded area of the periodic table to find out.

Order of sub-levels

What is the order of sub-levels in terms of energy?

3s  3d  4f  4s  4p  2p  4d  2s  3p  1s
**Shells, Orbitals & Sub-shells**

A **shell** is the set of all orbitals found in the **same energy level** (all have the same n-value)

- The second shell consists of the **2s and the 2p orbitals**

A **subshell** is a set of orbitals of the same type within a shell (or principal energy level)

- The set of three 2p orbitals in the second energy level (2pₓ, 2pᵧ, and 2pz)

---

**Where do the electrons go?**

<table>
<thead>
<tr>
<th>Types of Orbitals</th>
<th>n = 5:</th>
<th>4f</th>
</tr>
</thead>
<tbody>
<tr>
<td>s - type subshells contain</td>
<td></td>
<td></td>
</tr>
<tr>
<td>p - type subshells contain</td>
<td></td>
<td></td>
</tr>
<tr>
<td>d - type subshells contain</td>
<td></td>
<td></td>
</tr>
<tr>
<td>f - type subshells contain</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

---

Energy Level

1. 1s
2. 2s, 2p
3. 3s, 3p, 3d
4. 4s, 4p, 4d, 4f
The Aufbau principle

As part of his work on electron configuration, Niels Bohr developed the **Aufbau principle**, which states how electrons occupy sub-levels.

The Aufbau principle states that the lowest energy sub-levels are occupied first.

This means the 1s sub-level is filled first, followed by 2s, 2p, 3s and 3p.

However, the 4s sub-level is lower in energy than the 3d, so this will fill first.
Electron configuration & Energy Level Diagrams

Electrons fill lower energy sub-levels first.
*Although the 3d sub-level is in a lower principal energy level than the 4s sub-level, it is actually higher in energy.

All orbitals in the same energy level (same n value) have the same energy and are thus said to be degenerate orbitals.
This is only true for the hydrogen atom.

*Other polyelectronic atoms, have multiple electrons which repel each other, causing differences in energies between the subshells in a given energy level. (more on this later)

Writing electron configuration

Writing the electron configuration of an element

Writing out the electron configuration of an element shows how many electrons are in each sub-level.
Click "play" to find out how to do this.
**Electron configuration: true or false?**

<table>
<thead>
<tr>
<th>Statement</th>
<th>True/False</th>
</tr>
</thead>
<tbody>
<tr>
<td>1. Lithium has the electron configuration $1s^22s^1$.</td>
<td>?</td>
</tr>
<tr>
<td>2. Sulfur has the electron configuration $1s^22s^22p^4$.</td>
<td>?</td>
</tr>
<tr>
<td>3. Cl$^-$ and Ar both have the electron configuration $1s^22s^22p^63s^23p^6$.</td>
<td>?</td>
</tr>
<tr>
<td>4. Aluminium has the electron configuration $1s^22s^22p^63s^3$.</td>
<td>?</td>
</tr>
<tr>
<td>5. F$^-$ and N$^{3-}$ both have the electron configuration $1s^22s^22p^6$.</td>
<td>?</td>
</tr>
</tbody>
</table>

**Orbital Arrangements with the Periodic Table**

```
<table>
<thead>
<tr>
<th>2 e^-</th>
<th>10 e^-</th>
<th>6 e^-</th>
</tr>
</thead>
<tbody>
<tr>
<td>1s</td>
<td></td>
<td></td>
</tr>
<tr>
<td>2s</td>
<td>2p</td>
<td></td>
</tr>
<tr>
<td>3s</td>
<td>3p</td>
<td></td>
</tr>
<tr>
<td>4s</td>
<td>4d</td>
<td>4p</td>
</tr>
<tr>
<td>5s</td>
<td>5d</td>
<td>5p</td>
</tr>
<tr>
<td>6s</td>
<td>6d</td>
<td>6p</td>
</tr>
<tr>
<td>7s</td>
<td></td>
<td>7p</td>
</tr>
</tbody>
</table>
```

```
| 4f     |
```

```
| 5f     |
```
Example 1  
Silicon

Example 2  
Technetium

Practice: Predict the electron configurations for phosphorus, strontium, and cadmium.

Electron configuration of transition metals

Although the 3d sub-level is in a lower principal energy level than the 4s sub-level, it is actually higher in energy.

This means that the 4s sub-level is filled before the 3d sub-level.

Example: what is the electron structure of vanadium?

1. Count number of electrons in atom  23
2. Fill sub-levels, remembering 4s is filled before 3d  1s²2s²2p⁶3s²3p⁶4s²3d³
The electron configurations of chromium and copper are exceptions to the normal rules of orbital filling:

- **Chromium**:
  
  \[ 1s^22s^22p^63s^23p^64s^13d^5 \]

- **Copper**:
  
  \[ 1s^22s^22p^63s^23p^64s^13d^{10} \]

___ orbitals are more stable (i.e. have lower ________) when exactly half-filled or filled.

For this reason, an electron may be promoted from the ___ to the ___ in certain cases.

With larger atoms like this it can be useful to shorten the electron arrangement into core notation.

Copper can be shortened to [Ar]4s^13d^{10}. (called core notation)
Electron configuration of ions

- When writing the electron configuration of ions, it is important to add or subtract the appropriate number of electrons.
- Electrons in the outermost shell (largest n-value) are removed first.
- For non-transition metals, the sub-levels are then filled as for atoms.

For negative ions: add electrons.
For positive ions: remove electrons.

Example: what is the electron structure of O\(^2^-\)?

1. Count number of electrons in atom: 8
2. Add or remove electrons due to charge: 8 + 2 = 10
3. Fill sub-levels as for uncharged atom: 1s\(^2\)2s\(^2\)2p\(^6\)

Electronic configuration of transition metal ions

When transition metals form ions, it is the 4s electrons that are removed before the 3d electrons.

Example: what is the electron structure of Ni\(^2+\)?

1. Count number of electrons in atom: 28
2. Fill sub-levels, remembering 4s is filled before 3d: 1s\(^2\)2s\(^2\)2p\(^6\)3s\(^2\)3p\(^6\)4s\(^2\)3d\(^8\)
3. Count number of electrons to be removed: 2
4. Remove electrons starting with 4s: 1s\(^2\)2s\(^2\)2p\(^6\)3s\(^2\)3p\(^6\)3d\(^8\)
### Examples: Electron configuration of ions

1. **Negative Ions (Anions):** Add appropriate # of electrons to last subshell, starting with the configuration of the neutral atom.

   **Examples:**
   - $\text{O}^{2-}$
   - $\text{N}^{3-}$

2. **Positive Ions (Cations):** Uh, oh... there are some rules!
   - i) **the electrons in the outermost shell** (largest $n$-value) are removed first
   - ii) **after that, removal order is p before s before d** (within the outermost shell)

   **Examples:**
   - $\text{Sn}^{3+}$
   - $\text{Fe}^{3+}$

---

### Isoelectronic

**An adjective meaning:**

"has the same numbers of electrons as..."

**Example:**

Na$^+$ is isoelectronic to ______ since they both have ______ electrons
After a noble gas, a new period begins in the periodic table and so too, a **new energy level**. As we begin period 3, let’s represent the elements up to scandium in Table 5.4.2 using **electron configurations only**.

We can **condense electron configurations** using **core notation**, in which the configuration of the previous noble gas is **represented by that noble gas symbol in square brackets**, then outer electrons are indicated in **bold type**. This inner core contained full, closed shells, allowing the focus to be on the **valence electrons** above the core electrons in the **open outer shell**.

### Table 5.4.2: Electronic Configuration & Core Notation

<table>
<thead>
<tr>
<th>Element</th>
<th>Full Electron Configuration</th>
<th>Core Notation</th>
</tr>
</thead>
<tbody>
<tr>
<td>sodium</td>
<td>?</td>
<td>?</td>
</tr>
<tr>
<td>magnesium</td>
<td>?</td>
<td>?</td>
</tr>
<tr>
<td>aluminum</td>
<td>?</td>
<td>?</td>
</tr>
<tr>
<td>silicon</td>
<td>?</td>
<td>?</td>
</tr>
<tr>
<td>phosphorus</td>
<td>?</td>
<td>?</td>
</tr>
<tr>
<td>sulphur</td>
<td>?</td>
<td>?</td>
</tr>
<tr>
<td>chlorine</td>
<td>?</td>
<td>?</td>
</tr>
<tr>
<td>argon</td>
<td>?</td>
<td>?</td>
</tr>
<tr>
<td>potassium</td>
<td>?</td>
<td>?</td>
</tr>
<tr>
<td>calcium</td>
<td>?</td>
<td>?</td>
</tr>
<tr>
<td>scandium</td>
<td>?</td>
<td>?</td>
</tr>
</tbody>
</table>
Electron orbitals

It is *impossible to exactly locate* the position of an electron within an energy sub-level. By measuring the electron density around the nucleus, it is possible to define regions where electrons are most likely to be found at any one time. These regions are called **orbitals**.

Each **energy sub-level** has one or more orbitals, each of which can contain a **maximum of two electrons**.

<table>
<thead>
<tr>
<th>sub-level</th>
<th>no. orbits</th>
<th>max no. electrons</th>
</tr>
</thead>
<tbody>
<tr>
<td>s</td>
<td>1</td>
<td>2</td>
</tr>
<tr>
<td>p</td>
<td>3</td>
<td>6</td>
</tr>
<tr>
<td>d</td>
<td>5</td>
<td>10</td>
</tr>
<tr>
<td>f</td>
<td>7</td>
<td>14</td>
</tr>
</tbody>
</table>

Shapes of electron orbitals

**What are the shapes of electron orbitals?**

**Electron orbitals** are regions around the nucleus of an atom where there is a high probability of finding an electron.

All orbitals can hold a maximum of two electrons, but those in different sub-levels are different shapes and sizes.

Click a button on the right to see the shapes of some s and p orbitals.
Shapes of Atomic Orbitals

- Different atomic orbitals are denoted by letters.
- The s orbitals are spherical, and p orbitals are dumbbell-shaped.

- Four of the five d orbitals have the same shape but different orientations in space.

The Pauli exclusion principle and spin

The Pauli exclusion principle states that each orbital may contain no more than two electrons.

It also introduces a property of electrons called spin, which has two states: ‘up’ and ‘down’. The spins of electrons in the same orbital must be opposite, i.e. one ‘up’ and one ‘down’.

A spin diagram (or energy level diagram) shows how the orbitals are filled. Orbitals are represented by squares, and electrons by arrows pointing up or down.

spin diagram for magnesium, 1s²2s²2p⁶3s²
Rules for filling electrons

When two electrons occupy a p sub-level, they could either completely fill the same p orbital or half fill two different p orbitals.

Hund’s rule states that single electrons occupy all empty orbitals within a sub-level before they start to form pairs in orbitals.

If two electrons enter the same orbital there is repulsion between them due to their negative charges. The most stable configuration is with single electrons in different orbitals.

Evidence for Hund’s rule

The first ionization energies for the elements in period 3 show a general increase.

However, sulfur’s value is below that of phosphorus. As the highest energy electrons of both are in the 3p sub-level this is evidence for Hund’s rule.
Evidence for Hund’s rule: P vs. S

Phosphorus has three electrons in its 3p sub-level and sulfur has four.

The lower first ionisation energy for sulfur is because it has a pair of electrons in one of the 3p orbitals.

*Mutual repulsion between these two electrons makes it easier to remove one of them.*

<table>
<thead>
<tr>
<th>Element</th>
<th>3p</th>
<th>3s</th>
<th>2p</th>
<th>2s</th>
<th>1s</th>
</tr>
</thead>
<tbody>
<tr>
<td>Phosphorus</td>
<td>1↑</td>
<td>1</td>
<td>1↑</td>
<td>1</td>
<td>1↑</td>
</tr>
<tr>
<td>Sulfur</td>
<td>1</td>
<td>1↑</td>
<td>1↑</td>
<td>1</td>
<td>1↑</td>
</tr>
</tbody>
</table>

Creating spin diagrams

Creating electron spin diagrams

Click an element to start creating its spin diagram.
What's the point of all this stuff?

Valence Electrons are the electrons found in the outermost open shell of an atom.

- They are the ones that are able to take part in chemical reactions.
- Electrons in the core or in full d or f subshells are never valence electrons.

Review:

- For any atom, the **lowest energy state** refers to the situation where the electrons are in the lowest energy state possible. For hydrogen, this is when the electron is in the 1s orbital.
- When an electron is excited (absorbs energy) it will – depending on the amount of energy absorbed – jump up to any particular energy level above the ________________.
- In the hydrogen atom, all subshells in a given shell are ________________ (of equal energy). This is because there is only a single electron (no other repulsive forces). (e.g. energy of 2s = 2p)
- In multi-electron atoms, many orbitals are occupied simultaneously – the electrons “sense” each other through repulsive forces and have to be optimally arranged. In such atoms, subshells have different energies within each shell. (e.g. energy of 2s ≠ 2p)
- The listing of the electrons in the atom from lowest energy orbital to highest energy orbital is known as the **electron configuration** of an atom.
Electron Configuration Practice

Electron configurations for the first 18 elements:

<table>
<thead>
<tr>
<th>Element</th>
<th>Z</th>
<th>1s</th>
<th>2s</th>
<th>2p</th>
<th>3s</th>
<th>3p</th>
</tr>
</thead>
<tbody>
<tr>
<td>H</td>
<td>1</td>
<td>___</td>
<td>___</td>
<td>___</td>
<td>___</td>
<td>___</td>
</tr>
<tr>
<td>He</td>
<td>2</td>
<td>___</td>
<td>___</td>
<td>___</td>
<td>___</td>
<td>___</td>
</tr>
<tr>
<td>Li</td>
<td>3</td>
<td>___</td>
<td>___</td>
<td>___</td>
<td>___</td>
<td>___</td>
</tr>
<tr>
<td>Be</td>
<td>4</td>
<td>___</td>
<td>___</td>
<td>___</td>
<td>___</td>
<td>___</td>
</tr>
<tr>
<td>B</td>
<td>5</td>
<td>___</td>
<td>___</td>
<td>___</td>
<td>___</td>
<td>___</td>
</tr>
<tr>
<td>C</td>
<td>6</td>
<td>___</td>
<td>___</td>
<td>___</td>
<td>___</td>
<td>___</td>
</tr>
<tr>
<td>N</td>
<td>7</td>
<td>___</td>
<td>___</td>
<td>___</td>
<td>___</td>
<td>___</td>
</tr>
<tr>
<td>O</td>
<td>8</td>
<td>___</td>
<td>___</td>
<td>___</td>
<td>___</td>
<td>___</td>
</tr>
<tr>
<td>F</td>
<td>9</td>
<td>___</td>
<td>___</td>
<td>___</td>
<td>___</td>
<td>___</td>
</tr>
<tr>
<td>Ne</td>
<td>10</td>
<td>___</td>
<td>___</td>
<td>___</td>
<td>___</td>
<td>___</td>
</tr>
<tr>
<td>Na</td>
<td>11</td>
<td>___</td>
<td>___</td>
<td>___</td>
<td>___</td>
<td>___</td>
</tr>
<tr>
<td>Mg</td>
<td>12</td>
<td>___</td>
<td>___</td>
<td>___</td>
<td>___</td>
<td>___</td>
</tr>
<tr>
<td>Al</td>
<td>13</td>
<td>___</td>
<td>___</td>
<td>___</td>
<td>___</td>
<td>___</td>
</tr>
<tr>
<td>Si</td>
<td>14</td>
<td>___</td>
<td>___</td>
<td>___</td>
<td>___</td>
<td>___</td>
</tr>
<tr>
<td>P</td>
<td>15</td>
<td>___</td>
<td>___</td>
<td>___</td>
<td>___</td>
<td>___</td>
</tr>
<tr>
<td>S</td>
<td>16</td>
<td>___</td>
<td>___</td>
<td>___</td>
<td>___</td>
<td>___</td>
</tr>
<tr>
<td>Cl</td>
<td>17</td>
<td>___</td>
<td>___</td>
<td>___</td>
<td>___</td>
<td>___</td>
</tr>
<tr>
<td>Ar</td>
<td>18</td>
<td>___</td>
<td>___</td>
<td>___</td>
<td>___</td>
<td>___</td>
</tr>
</tbody>
</table>

How does this pattern of organizing electrons relate to the periodic table?

Summary of Quantum Numbers

Every electron can be uniquely described using four quantum numbers:

- **n** = principal quantum number – indicates the energy level. Bigger n-value means further from the nucleus.
- **l** = angular momentum quantum number – gives the shape of the orbital.
- **m** = magnetic quantum number – gives orientation of the orbital in space.
- **s** = spin quantum number – Tells you the orientation of the electron.

<table>
<thead>
<tr>
<th>Quantum number</th>
<th>Name</th>
<th>What it labels</th>
<th>Possible values</th>
<th>Notes</th>
</tr>
</thead>
<tbody>
<tr>
<td>n</td>
<td>principal</td>
<td>electron energy level or shell number</td>
<td>1, 2, 3, ...</td>
<td>Except for d-orbitals, the shell number matches the row of the periodic table.</td>
</tr>
</tbody>
</table>
| l              | azimuthal     | orbital type: s, p, d, f  | 0, 1, 2, ..., n-1 | 0 = s orbital  
1 = p orbital  
2 = d orbital  
3 = f orbital               |
| m_l            | magnetic      | orbital sub-type          | integers between and including  
-\( \ell \) and \( \ell \)  
-\( \ell \), \( -\ell +1 \), ..., \( -1 \)  
\( \ell \)  
\( \ell +1 \) in one orbital  
\( \ell +1 \) in each of three sub orbitals \( \ell \) in each of five sub orbitals \( \ell \) in each of five sub orbitals |  
\( \ell = 0 \) (s): 2 e\(^-\) in one orbital  
\( \ell = 1 \) (p): 2 e\(^-\) in each of three sub orbitals  
\( \ell = 2 \) (d): 2 e\(^-\) in each of five sub orbitals  
\( \ell = 3 \) (f): 2 e\(^-\) in each of five sub orbitals  
\( \ell = 4 \) (g): 2 e\(^-\) in each of five sub orbitals  
\( \ell = 5 \) (h): 2 e\(^-\) in each of five sub orbitals  
\( \ell = 6 \) (i): 2 e\(^-\) in each of five sub orbitals  
\( \ell = 7 \) (j): 2 e\(^-\) in each of five sub orbitals  
\( \ell = 8 \) (k): 2 e\(^-\) in each of five sub orbitals  
\( \ell = 9 \) (l): 2 e\(^-\) in each of five sub orbitals  
\( \ell = 10 \) (m): 2 e\(^-\) in each of five sub orbitals  
\( \ell = 11 \) (n): 2 e\(^-\) in each of five sub orbitals  
\( \ell = 12 \) (o): 2 e\(^-\) in each of five sub orbitals  
\( \ell = 13 \) (p): 2 e\(^-\) in each of five sub orbitals  
\( \ell = 14 \) (q): 2 e\(^-\) in each of five sub orbitals  
\( \ell = 15 \) (r): 2 e\(^-\) in each of five sub orbitals  
\( \ell = 16 \) (s): 2 e\(^-\) in each of five sub orbitals  
\( \ell = 17 \) (t): 2 e\(^-\) in each of five sub orbitals  
\( \ell = 18 \) (u): 2 e\(^-\) in each of five sub orbitals  
\( \ell = 19 \) (v): 2 e\(^-\) in each of five sub orbitals  
\( \ell = 20 \) (w): 2 e\(^-\) in each of five sub orbitals  
\( \ell = 21 \) (x): 2 e\(^-\) in each of five sub orbitals  
\( \ell = 22 \) (y): 2 e\(^-\) in each of five sub orbitals  
\( \ell = 23 \) (z): 2 e\(^-\) in each of five sub orbitals  |
| m_s           | spin          | electron spin             | ±\( \frac{1}{2} \) | Spins in any single sub-orbital must be paired. |
Homework

page 155 #26-27 (acegikmo), 28 (acegik), 29 (all)