

LEAVING CERTIFICATE CHEMISTRY

Catalytically

Cracking Chemistry

Higher and Ordinary Levels

Catherine Clayton



 **CJ Fallon**
ESTABLISHED 1895

**SAMPLE
CHAPTERS**

Table of Contents

Chapter 1	The Nature of Science
Chapter 2	Experimental Investigations
Chapter 3	The Kinetic Theory of Matter
Chapter 4	The Basics
Chapter 5	Physical & Chemical Changes
Chapter 6	Atomic Theory
Chapter 7	Electronic Configuration
Chapter 8	Chemical Bonding
Chapter 9	Shapes of Molecules & Intermolecular Forces
Chapter 10	The Periodic Table
Chapter 11	The Mole
Chapter 12	Gases
Chapter 13	Stoichiometry
Chapter 14	Solutions
Chapter 15	Rates of Reactions
Chapter 16	Acids & Bases
Chapter 17	Volumetric Analysis
Chapter 18	pH & Titration Curves
Chapter 19	Oxidation & Reduction
Chapter 20	Electrochemistry
Chapter 21	Chemical Equilibrium
Chapter 22	Introducing Hydrocarbons – The Alkanes
Chapter 23	More Hydrocarbons – The Alkenes & the Alkynes
Chapter 24	More Organic Families
Chapter 25	Thermochemistry
Chapter 26	Organic Reactions
Chapter 27	Organic Products
Chapter 28	Greenhouse Gases
Chapter 29	Water
Chapter 30	Modern Materials

CHAPTER 1

The Nature of Science (Model behaviour)

Can I...



Explain how scientists work (the scientific method)	
Appreciate how scientific ideas are changed over time	
Explain how science is a global enterprise that relies on evidence, communication, peer review and international conventions, repeatability and reproducibility	
Appreciate the role of chemistry in society (and its impacts on health, technology and sustainability)	
Appreciate how society influences scientific research	
Evaluate secondary sources of information, including those in the media	
Explain the term 'bias' and recognise bias in sources of information	
Present information (from personal research) on the contribution scientists make to scientific discovery and invention and its impact on society	
Discuss the use of models in chemistry	
Discuss the limitations of models	

1.1 The Nature of Science

The word science comes from the Latin word *scientia*, meaning 'knowledge'. Everything scientists do – research, carrying out experiments, collecting data – is all in the pursuit of knowledge. **The scientific method is a systematic, evidence-based approach that scientists use to gather, analyse and interpret data.** At the core of the scientific method lies the **testing of theories**. Examples of scientific theories you studied at Junior Cycle include the Big Bang, the theory of evolution, particle theory and collision theory.

A **scientific theory** is a hypothesis that has been verified by many different experiments and is widely accepted as the correct explanation.

Scientific theories set out to provide explanations that are consistent with the evidence and that can be tested. Scientific theories are different from scientific laws.

A **scientific law** is a statement that has been deduced from empirical evidence.

Empirical evidence refers to evidence gathered through first-hand observation, examination or experiments (rather than relying on abstract reasoning, theorising or speculating). Examples of laws include the law of conservation of mass (which we will study in Chapter 3) and Boyle's law (which we will study in Chapter 14).

A scientific law is different from a scientific theory as a theory sets out to provide an explanation as to how or why an aspect of nature behaves as it does, whereas a law describes what always happens under certain circumstances. **Laws do not change much unless an experimental error is discovered, while theories are always provisional or incomplete, and are refined and improved as new data becomes available.**

1.2 How scientific ideas are modified over time

Requiring evidence to support theories was not always the norm. For example, ancient Greek philosophers believed that everything was made of four elements (fire, air, earth and water), despite having no experimental evidence to support this idea. Nowadays, scientific theories are based firmly on evidence. Scientific knowledge is always evolving and developments in technology make new types of experiments possible. As new evidence is gathered, theories have to be altered or modified to take into account these advances in knowledge. For example, as new evidence emerged about the structure of the atom, the model of the atom had to be changed (many times, as we will see in Chapter 6).



Try It!

Research another three examples of how scientific theories changed as a result of new evidence.

1.3 Scientific method

The scientific method is a systematic, evidence-based approach that scientists use to gather, analyse and interpret data.

Scientists:

1. Make observations.
2. Develop and refine a research question.
3. Research.
4. Formulate a hypothesis.
5. Develop a testable prediction.
6. Design, plan and carry out an experiment to gather data.
 - The experiment must be a fair test.
 - Safety considerations must be taken into account.
 - Suitable equipment must be chosen.
 - Troubleshoot along the way – make changes if necessary.
 - Carry out the same experiment multiple times to ensure reliable, accurate results.
7. Analyse data.
8. Draw conclusions.
9. Accept or reject hypotheses.
10. Communicate results.



All of these steps will be covered in more detail in this chapter and in Chapter 2: Experimental Investigations.

The purpose of carrying out an experiment is to **find data to either support or reject a hypothesis. This process is rarely linear** – scientists often collect data, analyse it, identify errors, troubleshoot to determine the causes, redesign their methods, and repeat experiments as needed. **The process is as important as the product.**

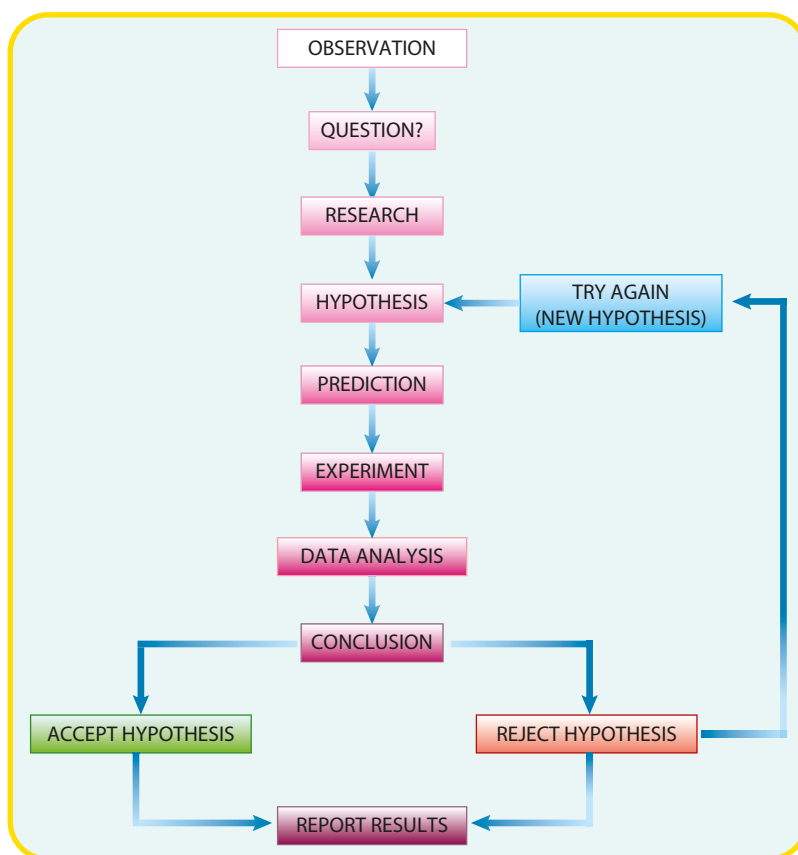


Figure 1.1

1.4 Science as a global enterprise

Science is a global enterprise in which scientists from all over the world collaborate to share knowledge, solve problems and advance our understanding of the world. This collaboration is essential, as scientific discoveries often build on the work of others. For example, during the Covid-19 pandemic, scientists worldwide worked together to develop vaccines. In order for scientists to successfully work together, science relies on evidence, clear communication, international conventions, peer review, repeatability and reproducibility.

Evidence

Scientific evidence is information and data collected through systematic observation, experimentation and analysis. It refers both to the information that we can gather from other scientists and the data from our own observations. Scientists must base hypotheses, experiments and conclusions on all of the available evidence, and must use this data in its entirety to support or reject a hypothesis. Gathering data selectively to suit a hypothesis is not science!

Clear communication

Scientists must be transparent and open about their work so that the global scientific community is able to evaluate their evidence and theories. It's important for scientists to publish their research so that others can learn from their work and build on it.

Scientists communicate in a variety of ways:

- Academic journals (e.g. *Nature*, *Science*, *New England Journal of Medicine*).
- Presentations at science conferences.
- Media (including social media).

Increasingly, more journals are becoming open-access journals (i.e. free, not behind a paywall). CORE and ScienceOpen are databases of open-access journal articles.



Try It!

Using CORE, ScienceOpen or another open-access journal, find an article on a topic you're interested in reading, and write down three new pieces of information that you have learnt.

International conventions

In science, the term 'international convention' has two meanings:

1. International convention can refer to **internationally agreed systems or standards**.
 - For example, SI units for measurement ensure that results from different parts of the world can be compared accurately.
 - The International Union of Pure and Applied Chemistry (IUPAC) has devised an international naming system for organic compounds.

International conventions such as these help maintain consistency in measurements, terminology, etc.

2. International conventions can also refer to **international agreements about a specific issue** – e.g. the 2015 Paris Agreement is an international agreement to keep the increase in the global average temperature to below 2°C above pre-industrial levels. It's part of the United Nations Framework Convention on Climate Change (UNFCCC).

Peer review

Peer review is the process by which scholarly work is evaluated by others working in the same field. This is typically the final point before an article is accepted for publication in a science journal.

The process begins when scientists conduct research (an experimental investigation or a different type of study – e.g. a survey) to gather data. After analysing their findings, they write a research article and submit it to a science journal. The editors of the journal may reject the article or, if considering publication, send the article to other scientists (working in the same field) for peer review. **Peer review involves other scientists reading the article, evaluating it and providing feedback to the editor.** They report on whether they think the article is original, methodical, well-argued, clearly written and important for the field.

If the article is not appropriate for publication, it's rejected. If it meets the required high standard, the editor provides feedback to the original scientist(s), who may make changes to the article before it's finalised and published. Although peer review is time-consuming, it's an **important safeguard** to ensure the validity and reliability of research and to protect against the spreading of inaccurate information.



Repeatability and reproducibility

Experiments should be both **repeatable and reproducible**.

Repeatable: Having obtained a result from an experiment, scientists can conduct the same experiment again, in the same location, with the same set-up, and produce the exact (or very similar) result. This must be done over a short period of time.

Reproducible: This refers to an entire experiment or study being reproduced by other scientists, who obtain the same results as the original scientists.

1.5 Conducting scientific research

Scientific research is a systematic process of investigating a specific question or problem in order to prove or disprove existing knowledge, discover new knowledge, and/or develop solutions to problems. It involves the collection, interpretation and evaluation of data.

Evaluating sources of information

One of the most important parts of research is choosing sources of information. To decide whether a secondary source is trustworthy, there are some features that you should consider (you can remember these by using the acronym **CARDS**):

C – Credibility: Is the source trustworthy? Does it come from a reputable journal, institution or organisation? Who are the authors? Are they experts in this field?

A – Accuracy: Are the claims backed by evidence? Is the data reliable, consistent and free from errors?

R – Relevance: Is the information directly related to your question or research?

D – Date: When was it published? Science evolves quickly, so older information may no longer be valid or accurate.

S – Sources: Are references provided? Reliable information cites evidence or secondary sources to back up claims.

It's also very important to establish if the source is **biased**.

Bias

Scientific bias refers to a lack of objectivity or a tendency to see or interpret evidence in ways that do not match what can be observed or concluded scientifically.

Bias can be **intentional or unintentional**, and can affect the methods chosen, the conclusions drawn or the way the research is reported. There are different types of bias. Some are described below.

- **Reporting bias:** Occurs when certain evidence is ignored or not reported.
- **Selection bias:** Occurs when a sample is chosen that doesn't represent the target population.
- **Confirmation bias:** Occurs when researchers focus only on information that supports their beliefs or expectations, and ignore other information.

- **Researcher bias:** Occurs when the personal views or interests of the researcher influence the outcome.
- **Social or cultural bias:** Bias due to the researcher's social or cultural points of view.



Test yourself

What type of bias is seen in the following examples?

1. A company wants to collect data from secondary school students but only surveys second-years.
2. A company funds a study to prove the safety of a product. The researcher conducting the study has shares in the company.
3. Sexist researchers are conducting a study on the abilities of women.
4. A scientist expects a drug to lower blood pressure. They focus only on the patients whose results show improvement, but ignore the patients whose results do not.
5. A researcher studying how effective a catalyst is publishes the data that shows positive results but not the data that contradicts this.

1.6 Science in the media

Most people do not read scientific journals. Often, the public hears about scientific breakthroughs in the media: newspapers, websites, radio reports, social media, etc. To analyse information in the media critically, you should use the same criteria you would to analyse a secondary source (i.e. CARDS; see section 1.5).

It's also important to be aware of pseudoscience. This refers to claims that are presented as scientific but are not backed up by rigorous scientific research (such claims are often based on anecdotal evidence). Also, ask yourself whether someone or some organisation stands to benefit from a claim – e.g. the tobacco industry has funded research into the benefits of smoking.



Try It!

Look up three recent articles that discuss scientific claims. Write an evaluation of each article using CARDS.

1.7 Impact of science on society

Scientific discoveries and inventions can have positive impacts on society – e.g. catalytic converters in cars reduce air pollution, water purification systems reduce illness from waterborne diseases, and pharmaceuticals treat diseases.

However, the impacts are not always positive. Scientific discoveries and inventions can also have negative impacts on society. For example, Fritz Haber developed the Haber process for synthesising ammonia for use in fertilisers that significantly improve crop yields and which have indirectly fed millions of people – this is often called 'the chemical reaction that feeds the



world'. However, fertilisers can also cause environmental problems, such as water pollution, particularly eutrophication (see Chapter 29).

Health

Chemistry has had a huge impact on human health and has been crucial to advances in disease prevention, diagnosis and treatment. Chemists play a role in almost every aspect of medicine: among other things they develop and synthesise new drugs, study how they act in the body and develop diagnostic and health screening techniques. Pharmaceuticals, many of which are derived from organic compounds, have revolutionised medicine, enabling the treatment and prevention of a wide range of diseases. Examples include aspirin, antibiotics and morphine (see Chapter 27). Chemists are also investigating the potential uses of carbon allotropes for drug delivery (see Chapter 30).

Water treatment and surfactants have also contributed positively to human health. Water treatment (see Chapter 29) provides clean, potable water which has drastically decreased illnesses and deaths due to waterborne diseases. Surfactants, such as soaps, have improved sanitation and helped prevent the spread of bacteria and viruses (see Chapter 27).

On the other hand, chemical reactions can also have negative consequences for health. Carbon dioxide emissions, for example, cause global warming (see Chapter 28), and chemicals in plastics and pesticides affect human and animal health. Medicines can have negative side effects, and chemical warfare is, of course, extremely dangerous.



Technology

Chemistry has also had a significant impact on technology. Lithium-ion batteries have been crucial in the development of renewable energy, of portable devices like smartphones, and of electric vehicles. New materials (e.g. fullerenes and carbon nanotubes) have enabled advancements in nanotechnology and electronics. However, there are drawbacks. Lithium-ion batteries, for example, are not environmentally friendly to produce, are difficult to recycle, and their improper disposal can cause environmental problems (see Chapter 30).



Sustainability

Chemistry also contributes to sustainability in multiple ways: chemists have developed environmentally friendly materials, energy-efficient processes, renewable alternatives to fossil fuels, and more advanced recycling techniques. Examples include the development of renewable fuels from biomass and agricultural waste (see Chapter 22), the development of hydrogen fuel cells that do not rely on fossil fuels (see Chapter 19), and the manufacturing of biodegradable plastics (see Chapter 27). New techniques for carbon capture and storage will be of increasing importance in combatting climate change (see Chapter 28).

As often, however, there is a downside. Some chemical processes and products undermine rather than contribute to sustainability efforts. Hazardous waste, pesticides, fertilisers, plastic pollution (including microplastics), habitat loss, ocean acidification, eutrophication and many other problems can be attributed, at least in part, to the work of chemists. Microplastics and ocean acidification will be discussed further in Chapter 29.



Research investigation 1

Research and present information on the contribution that scientists make to scientific discovery and invention, and their impact on society.

This research investigation should be filled in on pages ??–?? of your portfolio.

1.8 Impact of society on science

Often, society directly influences scientific research and scientists engage in research that reflects societal needs, challenges and priorities. A recent example of this is the development of Covid-19 vaccines. In January 2020, Chinese and Australian researchers, led by Zhang Yongzhen and Edward Holmes, published the genome of SARS-CoV-2 (severe acute respiratory syndrome coronavirus 2), which causes the respiratory illness Covid-19. They posted the genome – the genetic information of the virus – on Virological, an online platform for virologists, and this is widely regarded as a key factor in enabling the quick development of Covid-19 vaccines.

Currently, a significant global challenge to society is climate change. As we've just seen, scientific research is leading to the development of alternative fuel sources, techniques of carbon capture, and new, biodegradable materials.



Personal responsibility

If you want to be more effective in addressing the societal impact of science and technology, your first obligation is to be informed. Innovations are happening all the time and at great speed, so it's important to follow credible sources that will inform you of new developments. Try to stay up to date and to be aware, not just of what is happening but also of the implications that advances in science and technology have for society. Be aware of the ethical considerations sometimes raised by developments – e.g. the implications for privacy from the rise of AI, or considerations regarding the use of nuclear power. Being aware of big scientific issues like the urgency of combatting climate change should make you more willing to take personal responsibility wherever you can – e.g. participating in recycling initiatives, lobbying policymakers and reducing your carbon footprint.

1.9 Models

A **model** is a simplified representation of reality that is used to understand, explain or predict phenomena.



We use models all the time in everyday life to make sense of the world around us.

Everyday examples of models include:

- Maps, which are simplified representations of the real world. They help us to solve problems – e.g. planning a route and predicting distances. They use symbols to communicate information clearly and efficiently. Like all models, maps have limitations – e.g. a map in your geography book is static, while the real world is always changing.
- Weather models, which are used to predict the weather.
- Flight simulators (used by pilots) or driving simulators (e.g. used by Formula 1 drivers), which are models because they represent the performance and environment of a plane or car.

Models are also widely used throughout chemistry (and other sciences) to represent ideas, structures, processes or systems. **Diagrams, equations** (e.g. the ideal gas equation) and **simulations** are all examples of models. Models can also be more traditional – i.e. **physical models**, an example being the use of molecular modelling (molymod) kits to create molecules. We can make physical models of things that are too small to see, like molecules, or too large to see, like the solar system. Conceptual models are abstract and simplified representations that help understanding – e.g. Bohr's model of the atom.

Models can be used to describe and explain chemical phenomena as well as make predictions, test hypotheses, visualise concepts and solve problems – e.g. models used to predict the impacts of climate change. Models can also be used to predict the behaviour of a system or phenomenon. The periodic table is a model, and is used to predict trends in chemical behaviour and the properties of elements, such as their reactivity, ionisation energy and atomic radius, based on their position within the table (see Chapter 10).

Over the course of the next two years you will encounter models used to explain the behaviour of acids and bases (the Arrhenius model and Brønsted-Lowry model, Chapter 16), use the VSEPR model to predict molecular shapes (Chapter 9), describe concentration using the particle model (Chapter 14), model changing states using the kinetic theory of matter (Chapter 3), model Hess's law diagrammatically (Chapter 24), and model catalytic mechanisms (Chapter 15). You will study how models can be modified as more data becomes available (e.g. the model of the atom, Chapter 6), and how models use assumptions (model of an ideal gas, Chapter 12) and have limitations (e.g. collision theory, Chapter 15).

As more experiments are carried out and more data becomes available, models can be refined or modified. This is a fundamental part of science.

Limitations of models

All models have limitations:

- **Oversimplification:** Models often simplify complex systems by leaving out important details. This makes them easier to understand, but can make them less accurate. We must remember when using them that models are usually approximations.
- **Assumptions:** Many models make assumptions (which can lead to inaccuracies and errors).
- **Static vs dynamic:** Diagrams and physical models cannot accurately capture the dynamic, 3-D nature of molecules.

1.10 Chemical phenomena

Chemists (and you!) must be able to **relate observable phenomena** to the **chemical processes at the atomic, subatomic or molecular level** – i.e. link the macroscopic world with the microscopic. As you study chemistry over the next two years, you will see many examples of this. Table 1.1 gives a few.

	Macroscopic	Microscopic
Brownian motion	The pollen seems to be moving	Water molecules collide with the pollen grains, causing them to move randomly
Evaporation	The water 'disappears'	Water molecules gain enough energy to change state (liquid → gas)
Filtration	The residue is caught on the filter paper and the filtrate passes into the conical flask	We can visualise the residue and filtrate being made of particles: insoluble solid particles are unable to pass through the filter paper, while the liquid particles are able to pass through
Chemical reactions	A product is formed	Particles collide with sufficient energy and proper orientation, leading to effective collisions and reactions

Table 1.1

For more questions on the nature of science, see Chapter 1 in the accompanying skills book.

CHAPTER 6

Atomic Theory (Not so Bohr-ing!)

Can I...



Describe (and draw) the nuclear model of the atom

State the assumptions and limitations of the nuclear model of the atom

Describe (and draw) the Bohr model of the atom

State the assumptions and limitations of the Bohr model of the atom

Describe the orbital model of the atom

State the assumptions and limitations of the orbital model of the atom

Compare all three models of the atom

Describe (and draw) the shapes of the s and p orbitals

Bold = HL only

In the Junior Cycle you learnt that atoms are made up of protons, neutrons and electrons. You also learnt that the protons and neutrons are found in the nucleus, and that electrons are found in shells around the nucleus. But how do we know that this is what an atom looks like? And is this really the complete picture of an atom?

Many models of the atom have been put forward by scientists over the centuries. Studying some of these will help us to understand how scientists arrived at the modern structure of the atom and how scientists work (how they draw conclusions based on the experimental data they collect, and how they must be open to altering their ideas as new evidence emerges).

Note: You **don't need** to remember any dates given in this chapter – they're only for context. You also don't need to remember the names of scientists or the details of the experiments they carried out. These are included to aid your understanding, but the only content that can be examined in the LC exam is **the three atomic models and their assumptions and limitations**.

6.1 Nuclear model

Ernest Rutherford (1871–1937), a scientist from New Zealand, was working at the University of Manchester when he accidentally **discovered the existence of the nucleus**.

Rutherford's experiment

In 1909 Rutherford set out to investigate the structure of the atom. At the time scientists believed in what is called the plum-pudding model of the atom: they thought that the atom was essentially a sphere of positive charge with electrons embedded at random. Rutherford and his assistants set up an experiment in which a very thin sheet of gold foil was bombarded with alpha particles. Gold was chosen as it's very malleable and can be beaten into an extremely thin layer.



Alpha particles are a type of radioactive particle, and we now know (although Rutherford did not) that they consist of two protons and two neutrons.

Rutherford knew only that the alpha particles were positively charged, and he wanted to study the path of the positive alpha particles through the gold foil to investigate the structure of the atom.

Figure 6.1 shows the experimental set-up. A screen was set up to detect where the alpha particles hit after passing through the gold atoms.

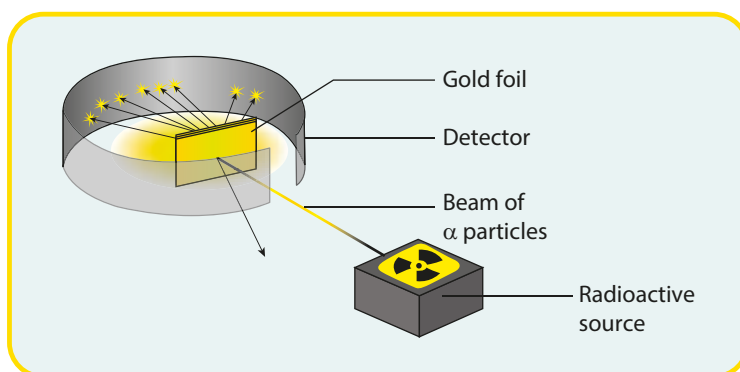


Figure 6.1

Basing their results on the plum-pudding model of the atom, Rutherford and his team expected the alpha particles to pass straight through the gold foil undeflected or to be slightly deflected when passing near an electron. Most alpha particles did pass straight through the gold foil undeflected (or slightly deflected), but some alpha particles were deflected at large angles and a very few alpha particles deflected straight back along their original paths.

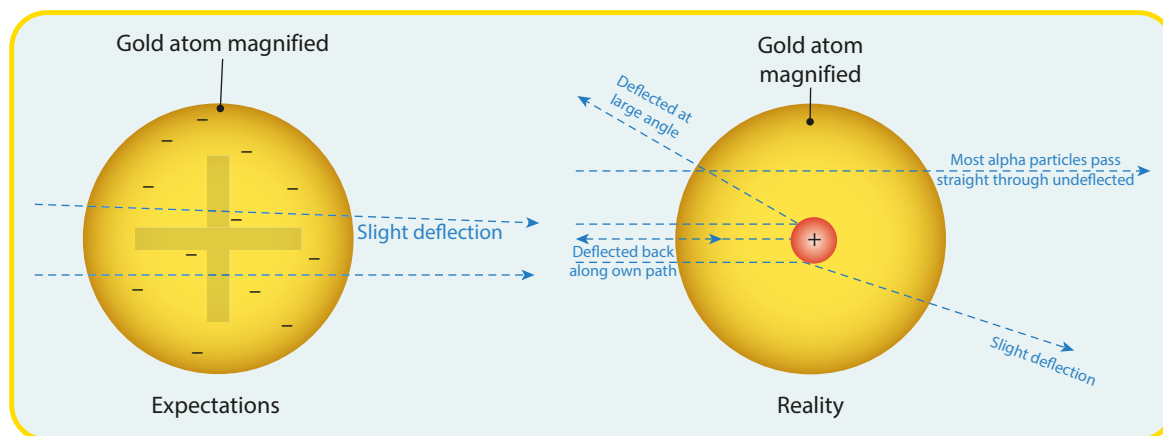


Figure 6.2

The nature of science

Rutherford anticipated that the alpha particles would simply pass straight through the gold foil with little to no deflection. However, being a meticulous scientist, he decided to place the detection screen all around the apparatus rather than just directly behind it, where he expected the alpha particles to be. This thoughtful approach led to unexpected results and serves as a valuable lesson in experimental design: scientists (and students!) must remain open-minded and prepared for unforeseen outcomes.



In 1911 Rutherford published his theory of the atom. It was based on the observations that he and his team made that led them to certain conclusions about the structure of the atom. (Table 6.1)

Observation	Conclusion
Most alpha particles passed straight through the gold foil undeflected	Most of the atom is made of empty space
Some alpha particles were deflected at large angles	There must be a positive centre, which he called the nucleus (like repels like, and since the alpha particles were positive they must have travelled near to, and been repelled by, something positive)
A few (as few as one in 20,000) alpha particles deflected straight back along their original paths	The positively charged nucleus must be very small and very dense (it must be small since so few alpha particles deflected back having collided with the nucleus, and it must be dense as it was able to deflect the alpha particles straight back)

Table 6.1

Based on these results, **Rutherford suggested a new model of the atom (the nuclear model)**, which had a very small, dense and positive core he called the nucleus. He suggested that the nucleus was surrounded by empty space within which electrons moved in wide orbits. However, his theory was unclear on where exactly electrons were to be found and what they were doing. (Figure 6.3)

Assumptions of the nuclear model

- The nucleus contains most of the atom's mass
- Electrons orbit around the nucleus in a relatively empty space

Limitations of the nuclear model

- Lacks detail about electron behaviour and doesn't clearly explain electron arrangement

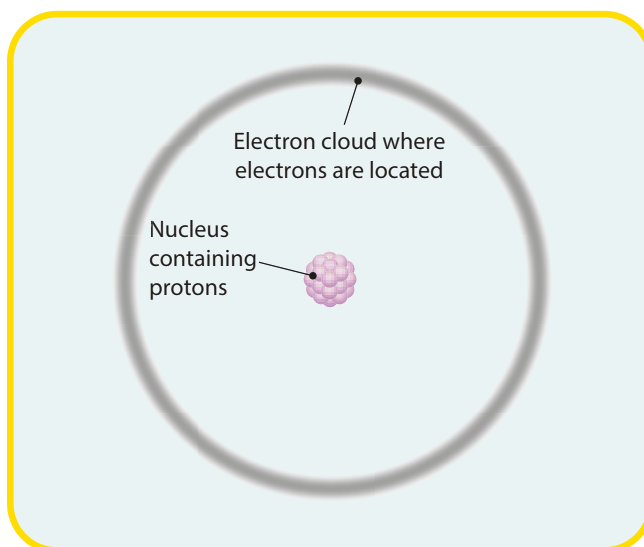


Figure 6.3 Diagram



Link it

The next atomic model we study is Bohr's model of the atom. Before reading on, can you describe the structure of Bohr's model of the atom? (It is the one you are familiar with from JC).

6.2 The Bohr model

In 1913 Niels Bohr (a Danish scientist) built on Rutherford's work and proposed his **planetary model** of the atom. From his study of the atomic emission spectrum of hydrogen (which we will study in detail in Chapter 7), Bohr proposed that in an atom of hydrogen the single electron orbits the nucleus (similar to how planets orbit the Sun).

However, the crucial difference between Rutherford's model of the atom and Bohr's was that Bohr proposed that **electrons in an atom have a specific, fixed amount of energy** (a quantum of energy), and so can move around the nucleus only in **certain specific orbits** with a fixed radius, depending on the fixed amount of energy they have. This was the first time this had been suggested and it revolutionised the world of science (and contributed to the emerging theory of quantum mechanics).

Bohr's theory states that electrons are found in **energy levels**. Electrons in the first energy level – the closest to the nucleus – have the same amount of energy as each other, and that amount of energy is less than the energy of electrons in the second energy level (further from the nucleus). Bohr represented energy levels using the letter n : $n = 1$ for the first, $n = 2$ for the second, $n = 3$ for the third (more about this in Chapter 7).

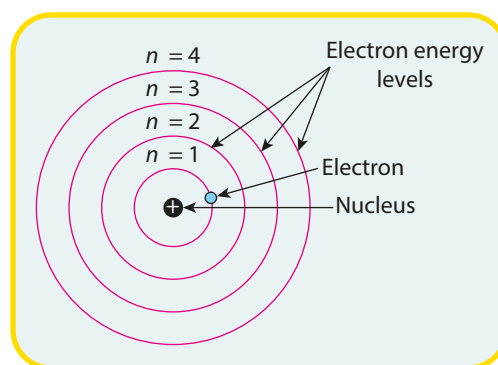


Figure 6.4

An **energy level** is the fixed amount of energy of an electron in an atom.

However, although Bohr's model of the atom worked well for hydrogen, **it didn't work so well for atoms containing more than one electron** (multi-electron atoms). This was due to some limitations of his theory.

Limitations of Bohr's model of the atom

- Bohr's theory didn't take into account wave-particle duality (see Table 6.2)
- We now know that electrons don't travel in fixed orbits, but rather are found in orbitals (due to Heisenberg's uncertainty principle we can refer only to the probability of finding an electron) (see Table 6.2)
- Bohr's theory didn't account for sublevels (you will learn about sublevels on page ??)

Further work on atomic theory

Continued work by Rutherford, and work by many other scientists – Broglie, Schrödinger, Heisenberg and Chadwick among them – led to a new model (the current model) of the atom: the orbital model. It's helpful to have a basic idea of how each of these scientists contributed to developing our understanding of the atom, resulting in our current model.



Ernest Rutherford	Discovered the existence of the proton and concluded that protons were present in the nucleus of all atoms
Louis de Broglie	Proposed that particles have wave-particle duality: they can behave both as particles and waves – see Figure 6.5. (therefore, Bohr's picture of them travelling in a precise orbit at a precise distance from the nucleus is not entirely correct)
Erwin Schrödinger	Schrödinger used mathematical equations to predict where electrons are located within the atom. He identified regions of the atom where electrons had a high probability of being found. These regions are called orbitals and are of various shapes – e.g. spherical and dumb-bell shaped. (Again, this conflicted with Bohr's idea of electrons travelling in circular orbits.)
Werner Heisenberg	Heisenberg's uncertainty principle states that it is impossible to measure both the velocity and the position of an electron at the same time
James Chadwick	Discovered the existence of the neutron

Table 6.2

6.3 The orbital model

When Schrödinger's wave equations were solved, four kinds of 3-D space were detected (in contrast to Bohr's 2D energy levels), within which there is a very high probability of finding an electron of specific energy. These regions of space were called orbitals, and the four types named s, p, d and f.

An **orbital** is a region of space around the nucleus of an atom within which there is a high probability of finding an electron.

S orbitals are spherical, with the nucleus at their centre. Each energy level has an s orbital – e.g. 1s, 2s – and the size of the orbital is dependent on the energy level to which it belongs.

P orbitals are dumb-bell shaped, arranged around the central nucleus. There are three kinds of p orbitals – p_x , p_y and p_z , oriented at right angles to each other, as shown in Figure 6.7.

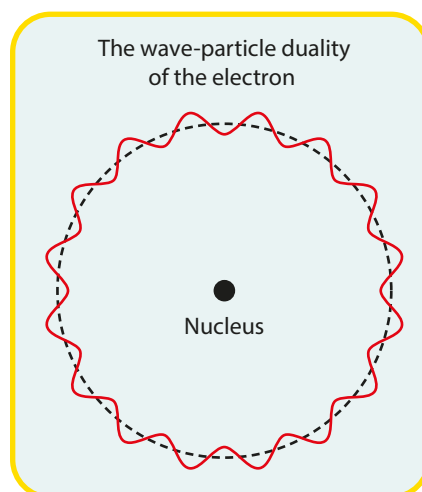


Figure 6.5

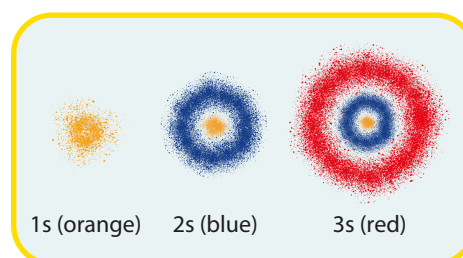


Figure 6.6

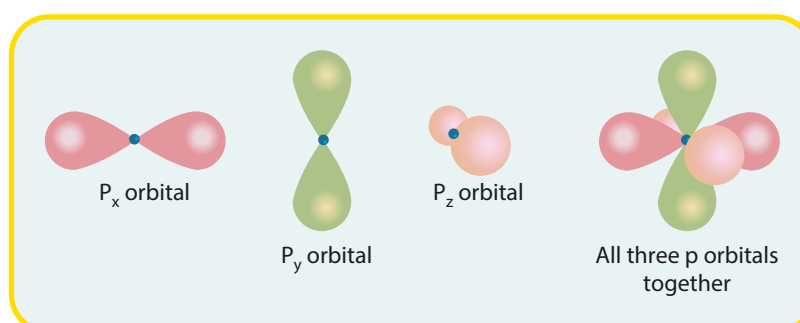


Figure 6.7

When s and p orbitals are mapped together, an atom that looks like Figure 6.8 is shown. These orbitals surround the nucleus, which is tiny but very dense, and is home to both protons and neutrons. (You will study orbitals in more depth in Chapter 7.)

The orbital model of the atom is actually much less specific than some of the previous models proposed – we can't state exactly both the position and speed of electrons, and we cannot even state the exact size of an atom.

If you find it odd to imagine an electron behaving as both a particle and a wave, and odd that we can talk only about regions where there is a high probability of finding an electron, you are not alone. As Bohr said, 'those who are not shocked when they first come across quantum theory cannot possibly have understood it'.

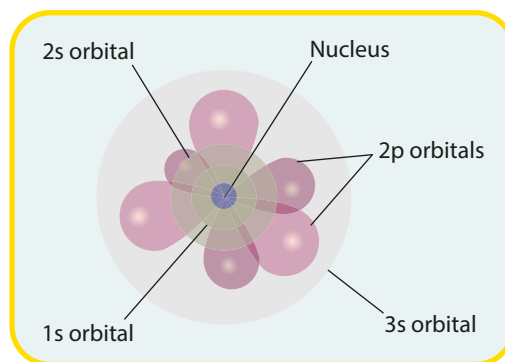


Figure 6.8

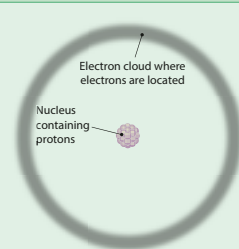
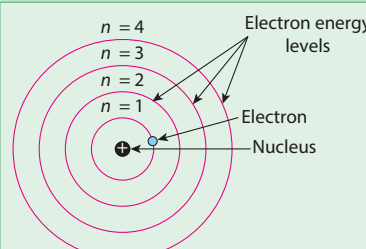
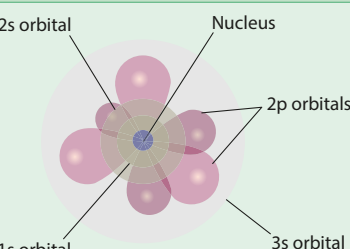
Model of the atom	Nuclear model	Bohr model	Orbital model
Diagram			
Assumptions	<p>The nucleus contains most of the atom's mass</p> <p>Electrons orbit around the nucleus in a relatively empty space</p>	<p>Bohr assumed that electrons had fixed amounts of energy and could occupy only certain energy levels</p> <p>Bohr assumed that electrons travelled in specific orbits around the nucleus</p>	<p>Electrons are found in orbitals – regions of space where there is a high probability of finding an electron</p> <p>Electrons have wave-particle duality.</p>
Limitations	<p>Lacks detail about electron behaviour and does not explain electron arrangement.</p>	<p>Bohr's model worked well for hydrogen, but not for more complex atoms</p> <p>Bohr's model didn't take into account wave-particle duality</p> <p>Bohr mistakenly believed that the exact position of electrons could be known at all times (contrary to Heisenberg's uncertainty principle)</p> <p>Bohr's model didn't account for sublevels</p>	<p>We can predict only the likelihood of where electrons are – we do not know their exact positions</p>

Table 6.3



The nature of science

How scientific ideas are modified over time

The study of atomic theory is a very good opportunity for us to realise how experimental evidence informs scientific thinking. As a result of experimental evidence, the accepted scientific theory had to change. As we know, this is an important part of science: **the ability to revise theories based on new evidence and the ability to devise experiments that test the work of previous scientists.**

How scientists work

As we trace the path of atomic theory we can see that many scientists lead us to our current understanding of atomic structure. **It's important to note that these scientists worked collaboratively – building on, and learning from, each others' work** – e.g. Bohr and Chadwick worked with Rutherford, and Heisenberg worked with Bohr.



Test yourself!

1. (a) Draw labelled diagrams of the (i) nuclear model of the atom; (ii) Bohr model of the atom; (iii) orbital model of the atom. (b) Distinguish between these three models in terms of the location of electrons.
2. What limitations of the nuclear model of the atom led to the development of Bohr's model?
3. Compare the nuclear model to the current atomic model. In what ways does the nuclear model remain relevant today, and what are some of the issues with this model?
4. Why is it important for scientists to evaluate and refine atomic models over time?
5. In what way is the orbital model less specific than other models of the atom?
6. Explain one assumption and one limitation of (a) Bohr's model of the atom; (b) the orbital model of the atom.

For more questions on atomic theory, see Chapter 6 in the accompanying skills book.

CHAPTER 7

Electronic Configuration (Don't be negative!)

Can I...



Write the electronic configuration of elements 1-20 showing electrons present in main energy levels

Write the electronic configuration of ions of the elements 1-20 showing electrons present in main energy levels

Explain the origin of lines on the atomic emission spectrum of hydrogen

Define the following terms: electron transition, photon energy, photon frequency, ground state, excited state

Explain the equation $E_m - E_n = hf$

Identify an element using flame tests (Experiment 2)

Identify a cation in an unknown salt (Experiment 2, EI)

Identify Na, Sr, Cu from their emission line spectra

Write the electronic configuration of elements 1-36 showing electrons present in main energy levels, sublevels and orbitals

Write the electronic configuration of the ions of elements 1-36 (excluding transition metal ions)

Bold = HL only

Note: This chapter contains mostly HL material so the OL material will be covered first (pages ??-??). The rest of the chapter is HL only, except for the experiment to identify elements on page ??, which must be completed by all students.

7.1 Simple electronic configurations

Writing electronic configurations (including main energy levels only)

The arrangement of electrons in an atom is called its electronic configuration. As discussed in Chapter 6, the Bohr model of the atom isn't entirely correct. However, the Bohr model is still useful for writing simple electronic configurations for the first twenty elements, when focusing only on the electrons in the principal energy levels (shells). To write simple electronic configurations correctly, remember that the first energy level can hold a maximum of two electrons, while the second and third can hold a maximum of eight electrons. (This isn't strictly true for the third energy level, but will work for simple electronic configurations).



Element	Atomic number	Electron configuration
Hydrogen	1	1
Helium	2	2
Lithium	3	2,1
Beryllium	4	2,2
Boron	5	2,3
Carbon	6	2,4
Nitrogen	7	2,5
Oxygen	8	2,6
Fluorine	9	2,7
Neon	10	2,8
Sodium	11	2,8,1
Magnesium	12	2,8,2
Aluminium	13	2,8,3
Silicon	14	2,8,4
Phosphorus	15	2,8,5
Sulfur	16	2,8,6
Chlorine	17	2,8,7
Argon	18	2,8,8
Potassium	19	2,8,8,1
Calcium	20	2,8,8,2

Writing electronic configurations of ions (main energy levels only)

You must also be able to write electronic configurations for ions (simple ions only, not polyatomic ions). As you know, ions are atoms that have lost or gained electrons.

Example 1

Write the electronic configuration of the ion Mg^{2+} .

A magnesium atom has twelve electrons, with an electronic configuration of 2,8,2. The 2+ sign tells us that two electrons have been lost from the atom, so now there are ten electrons left (2,8). However, this is also the electronic configuration of an atom of neon.

To distinguish between ...

Ne 2,8

Mg^{2+} 2,8

... we can use [] and the charge to indicate that it is an ion:

$\text{Mg}^{2+} = [2,8]^{2+}$



Example 2

Write the electronic configuration of the ion Cl^- .

A chlorine atom has seventeen electrons, with an electronic configuration of 2,8,7. The minus sign tells us that the atom has gained one electron, so now there are eighteen electrons (2,8,8). However, this is also the electronic configuration of an atom of argon.

To distinguish between ...

Ar 2,8,8

Cl^- 2,8,8

... we can use [] and the charge to indicate that it is an ion:

$\text{Cl}^- = [\text{2,8,8}]^-$

For those studying HL chemistry, you must be able to write more detailed electronic structures that give more information about the exact arrangement of electrons. First, however, we will study the emission spectrum of hydrogen as this will give us a clearer understanding of how Bohr developed his model of the atom (which we learnt about in Chapter 6). Then we will look at how scientists discovered the existence of sublevels and learn more about the orbitals plotted mathematically by Schrödinger. We will then use this new knowledge to write electronic configurations that include energy levels, sublevels and orbitals.

HL

7.2 Continuous spectra

Light travels in waves. When white light (also known as visible light) is separated into its different wavelengths, a continuous spectrum of colours can be observed. A continuous spectrum is the band of colours produced when light is separated into its components; a rainbow is an example. A prism – a block of glass with a triangular cross-section – can be used for this separation. Light waves are refracted (bent) as they enter and leave the prism. (Figure 7.1)

Since different colours of light have different wavelengths, they have different degrees of refraction – i.e. they 'bend' by different amounts, causing the colours to be seen separately. The shorter the wavelength of the light, the more it is refracted. At one end of the spectrum is red light, which is refracted the least, and at the other end is violet light, refracted the most. (Rainbows are caused when raindrops or mist acts as a prism for sunlight.)

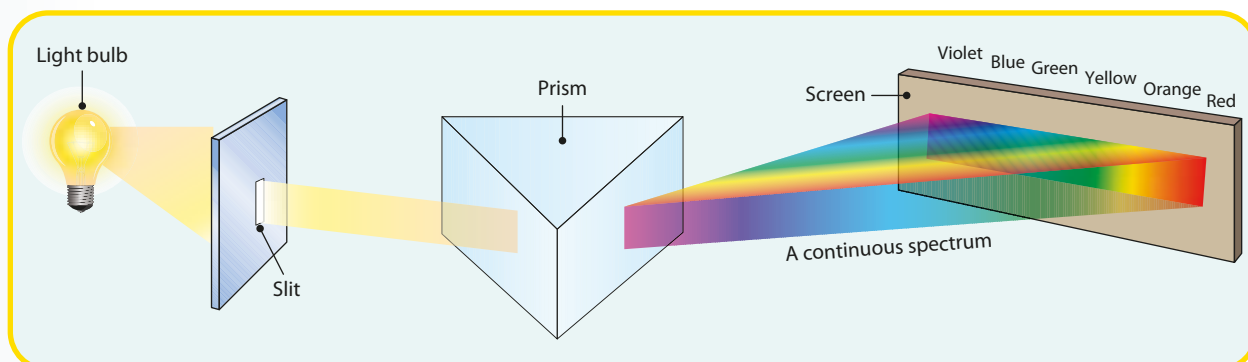


Figure 7.1

7.3 Line emission spectra

If we repeat the experiment shown in the diagram above using a discharge tube filled with hydrogen gas (a tube of hydrogen gas that has an electric current passed through it), we no longer see a continuous spectrum. Instead, we see a line spectrum of specific colours (Figure 7.2). This is called a **line emission spectrum**. Spectra are studied using a machine called a **spectrometer**.

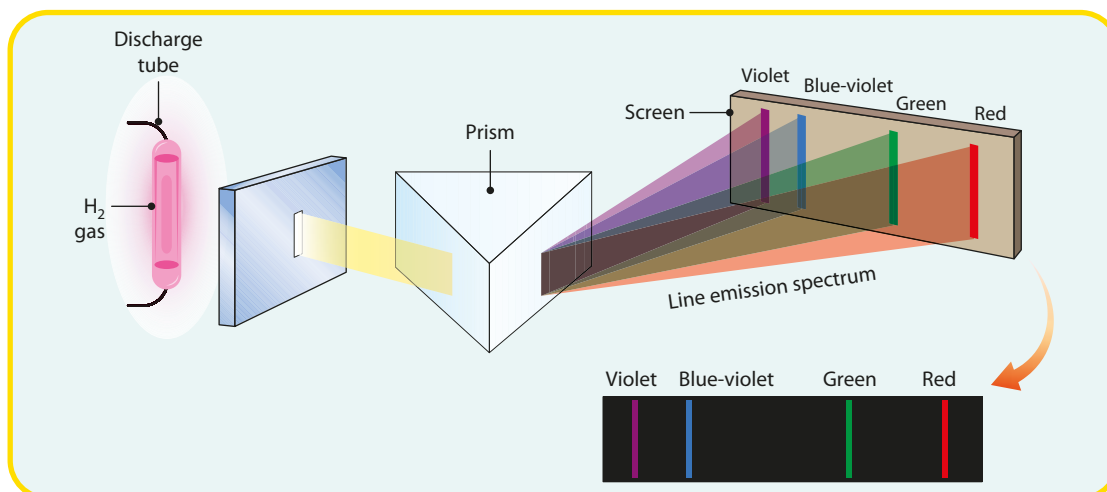


Figure 7.2

When this is repeated with different elements, different line spectra are obtained.

Each element has its own unique line spectrum (in the same way that each item in a supermarket has its own unique barcode). Studying the emission spectrum of hydrogen led Bohr to develop his model of the atom. He wanted to create a model of the atom that explained how line emission spectra occurred, and why they are unique to each element.

How do line emission spectra arise?

Bohr's theory is as follows: the lines appearing on the hydrogen spectrum are due to **electron transitions between energy levels**.

An **energy level** is the fixed amount of energy of an electron in an atom.

Atoms normally exist in the **ground state**, as this is the most stable.

The **ground state** of an atom is one in which the electrons occupy the lowest available energy levels.

The lowest energy level is the one closest to the nucleus and is called $n = 1$, the next is $n = 2$, etc. Electrons in these energy levels have fixed, 'quantised', amounts of energy.

Quantised energy means that the electrons can have only certain specific energy values. Values between the quantised values are not allowed.

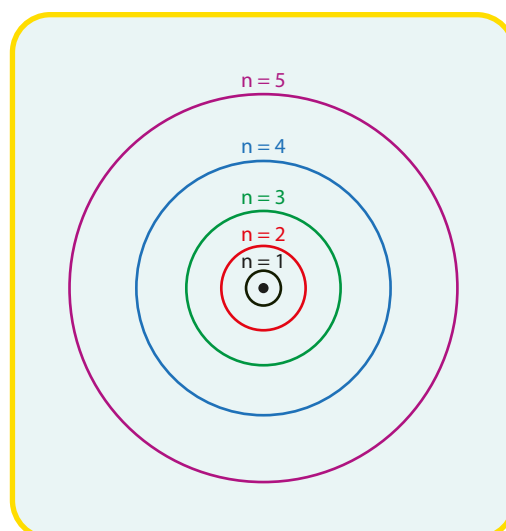


Figure 7.3



When an atom receives the right amount of energy (e.g. when it is **heated** or when electricity is passed through it), **energy is absorbed**. If the **energy absorbed by an electron is equal to the difference in energy between energy levels**, electrons can use this energy to **jump from lower energy levels to higher energy levels**. This is called an **electron transition** (the electron has moved from one energy level to another). The electrons are now **excited**. (Note: If the energy absorbed is not equal to the difference in energy between energy levels, then no electron transition takes place.)

The **excited state** of an atom is one in which the electrons occupy higher energy levels than those available in the ground state.

Electrons in the excited state are **unstable** and can't remain in the higher energy level – i.e. they fall back down to their original lower energy level (either in one transition or several – this is called electron relaxation).

As they fall back down, electrons **release energy in the form of a photon of light**. The energy released is the **difference in energy between the higher energy level and the lower energy level**. Since the electron is falling back down to a fixed energy level, only fixed amounts of light can be given off – **light of a definite frequency**. This specific frequency of light **corresponds to a particular colour**, which is the colour that appears on the line emission spectrum.

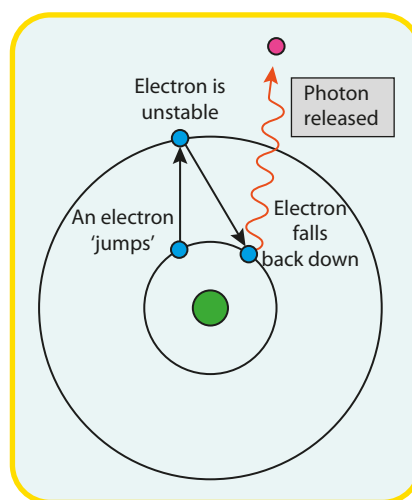


Figure 7.4

7.4 Photons

Photons are often described as 'packets' of energy. Photons are a quantum of electromagnetic energy – the smallest possible 'packet' or 'piece' of electromagnetic energy. Electromagnetic energy refers to energy that is transmitted in waves that travel at the speed of light in a vacuum (some examples are microwaves, radio waves, visible light waves, UV (ultra violet) rays, x-rays, gamma rays). Of these, the only electromagnetic waves visible to the human eye are those within the visible light spectrum (the term 'photon' comes from the Greek word 'photos', meaning light). **Photons exhibit wave-particle duality (can act as both a particle and a wave) and have a wavelength and a frequency.**

Photon energy is the energy of a single photon. It is proportional to the frequency of a photon.

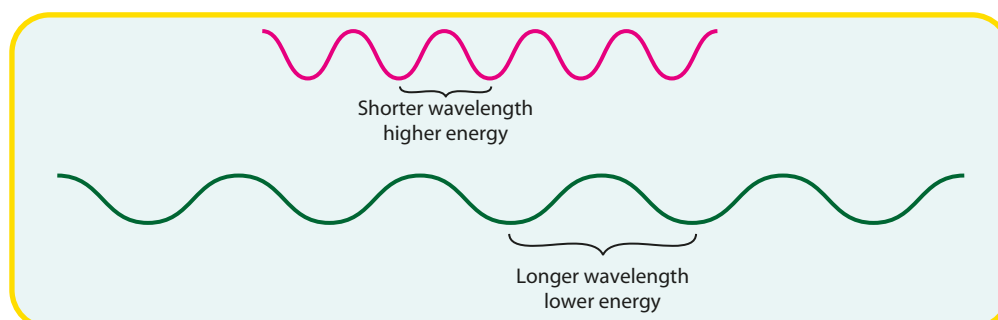


Figure 7.5

As can be seen in Figure 7.6, the peak of a wave is called its crest. The dip of a wave is called the trough. The distance between crests is called the wavelength. The frequency of a wave is the number of crests that pass a given point per second.

The **frequency** of a photon is defined as how many wavelengths a photon propagates per second.

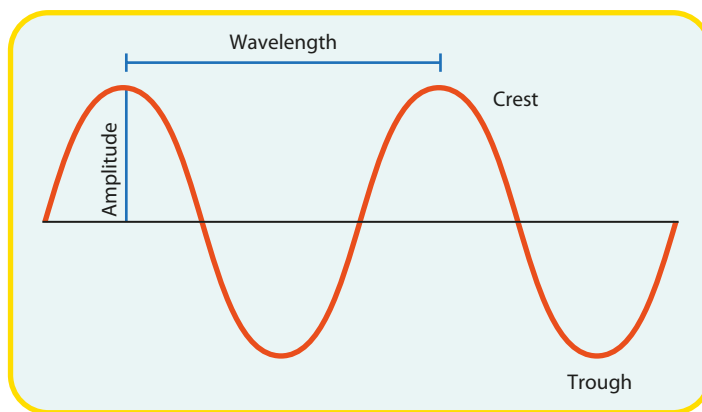


Figure 7.6

The frequency of light released can be calculated using the formula $E_m - E_n = hf$ where

E_m = the energy of the higher energy level (that the electron jumps to)

E_n = the energy of the lower energy level (that the electron falls back down to)

h = Planck's constant

f = frequency of the photon (frequency of emitted light)

The higher the photon's frequency, the higher its energy. Higher energy photons have shorter wavelengths. The lower the photon's frequency, the lower its energy. Lower energy photons have longer wavelengths. The frequency and wavelength of a photon determine the colour observed in the line emission spectrum.



Crack It! – Bohr's theory

- Atom is in the ground state – the electrons occupy the lowest available energy levels.
- Energy is supplied – e.g. the atom is heated.
- If the energy supplied is equal to the difference in energy levels, electrons will use this energy to jump to a higher energy level.
- Electrons are now excited but also unstable.
- Electrons drop back down to lower energy levels.
- As electrons fall they emit energy as photons of light.
- The frequency of light emitted is equal to the difference between the two energy levels ($E_m - E_n = hf$).
- The higher the photon's frequency = the higher the energy = the shorter the wavelength.
- The lower the photon's frequency = the lower the energy = the longer the wavelength.
- The light emitted appears as a specific colour on the line emission spectrum.



7.5 Hydrogen emission spectrum

Figure 7.7 shows the emission spectrum of hydrogen.

The visible lines on the hydrogen emission spectrum occur as a result of the following transitions:

- The **violet** line occurs due to electrons falling from **$n = 6$ to $n = 2$** .
- The **blue-violet** line occurs due to electrons falling from **$n = 5$ to $n = 2$** .
- The **blue-green** line occurs due to electrons falling from **$n = 4$ to $n = 2$** .
- The **red** line occurs due to electrons falling from **$n = 3$ to $n = 2$** .

Remember that any sample of hydrogen used to create an emission spectrum contains millions of atoms of hydrogen. Despite hydrogen having only one electron, four lines appear on its emission spectrum. This is because in some atoms the electron will jump to $n = 3$, in others to $n = 4$, etc.

The lines occurring in the **visible region** of the hydrogen spectrum are called the **Balmer series**. The Balmer series are the lines created when a hydrogen electron transitions **from a higher energy level down to $n = 2$** .

Not all of the lines appearing in the hydrogen emission spectrum are in the visible part of the spectrum. The hydrogen emission spectrum also has ultra-violet (UV) and infrared lines, which can be detected using machines.

The **Lyman series** contains lines in the **UV region** of the spectrum, and are caused by **electrons falling to $n = 1$** . The **Paschen series** contains lines in the **IR portion** of the hydrogen spectrum that are caused by electrons falling from higher energy levels **to $n = 3$** .

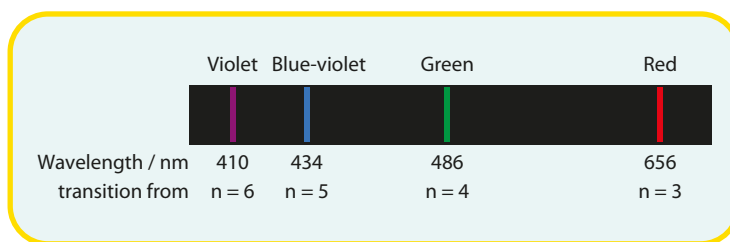


Figure 7.7

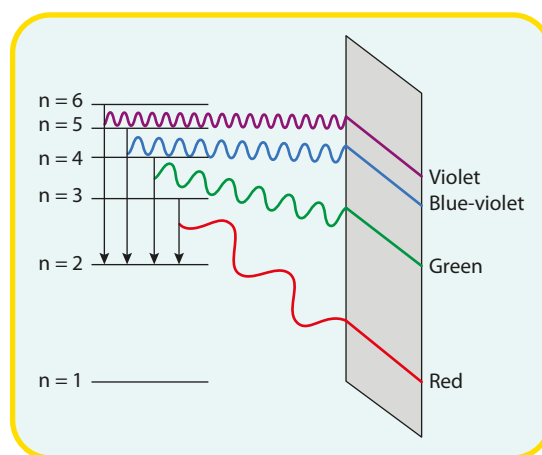


Figure 7.8



Crack It!

Electrons falling to $n = 1$ emit UV light = Lyman series

Electrons falling to $n = 2$ emit visible light = Balmer series

Electrons falling to $n = 3$ emit IR light = Paschen series

Bohr's theory worked well to explain the line emission spectrum of hydrogen. However, Bohr's theory couldn't satisfactorily explain emission spectra of other elements (where atoms contain multiple electrons, the effect of the electrons on each other has to be taken into account, which Bohr didn't do). Bohr's theory also had other limitations: as we know from Chapter 6, it didn't



HL

take into account the wave nature of the electron or sublevels (since Bohr wasn't aware they existed), and his theory contradicted Heisenberg's uncertainty principle.

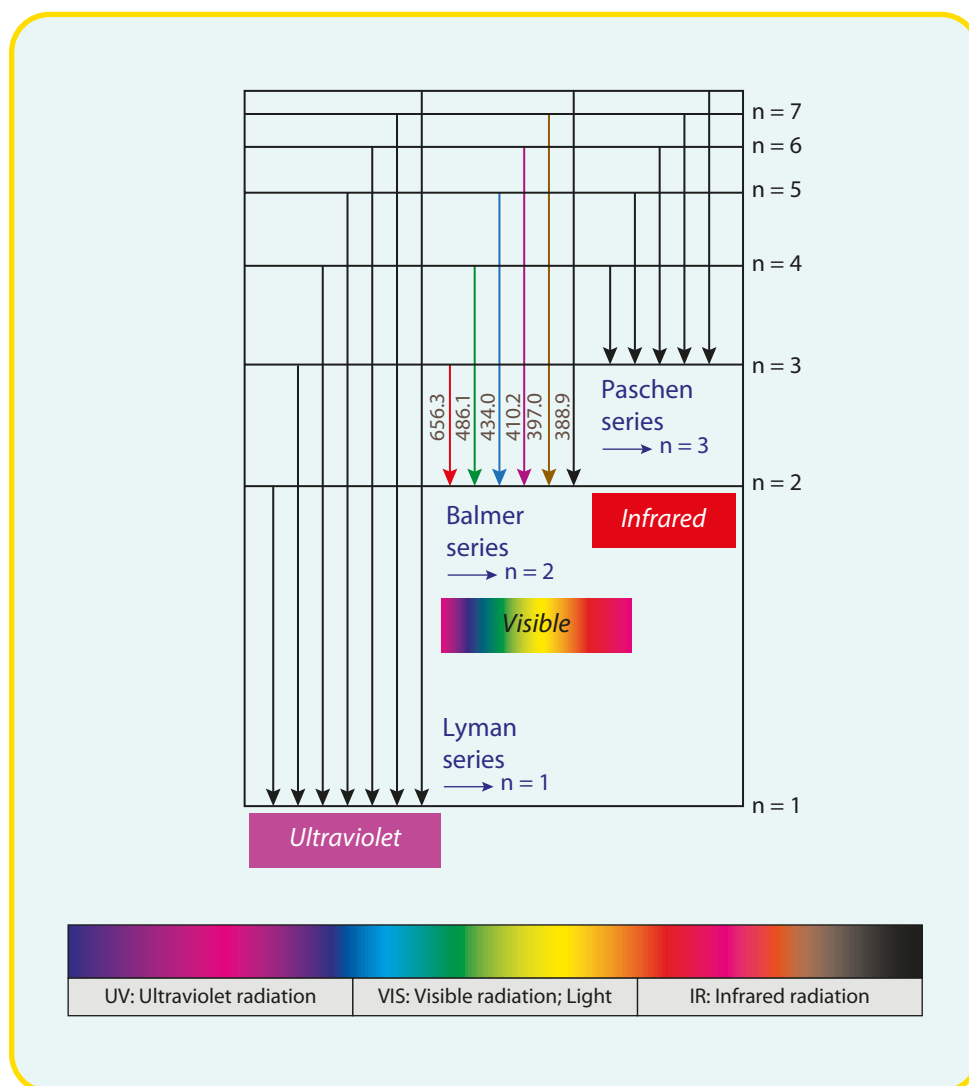


Figure 7.9

So what are sublevels and how did scientists discover them? We will find out in just a moment. Before we do, it's time to carry out an experiment to learn how to identify elements using flame tests and line emission spectra.

Experiment 2: Identifying elements using flame tests

The full method for this experiment is on page ?? of your portfolio. This should be carried out before reading the following information.

Part 1: Flame tests

This investigation is about identifying elements using primary and secondary data through (Part 1) conducting flame tests and (Part 2) studying line emission spectra.



Wooden splints are soaked overnight in water. A small amount of each salt (e.g. KCl) is crushed using a pestle and mortar. The wooden splint is dipped into the crushed salt and then held in the blue flame of a Bunsen burner. (The blue flame is used since it's hotter than the yellow and ensures enough energy is provided for electrons to 'jump' to higher energy levels. It also allows for clearer and more distinct observation of the colours produced by the salts). Note the colour produced. Repeat for all salts using separate pestle and mortars and separate wooden splints.

Element	Colour flame
Potassium	Lilac
Sodium	Yellow
Copper	Blue-green
Lithium	Crimson
Barium	Yellow-green
Strontium	Red (scarlet)

Different colour flames produced by different elements are the results of electron transitions. As they are heated, electrons absorb energy equal to the difference between two energy levels, and use it to jump from lower energy levels to higher energy levels. As electrons fall back down to the lower energy levels, photons of light are emitted. This light corresponds to the observed colour flame. (We have already discussed a detailed explanation of this on page ??.)

Part 2: Line emission spectra

You must be able to identify three elements from their line emission spectra – sodium, strontium and copper. They all have unique features that make them distinguishable from each other.

Sodium

Sodium's emission spectrum is easily identifiable by its **characteristic bright-yellow doublet**. This doublet consists of two very closely spaced lines at wavelengths of approximately 589.0 nm and 589.6 nm (nm refers to nanometres, which are equal to one-billionth of a metre – they are the unit of measurement for visible light).

These **yellow** lines are commonly known as the '**sodium D-lines**', and they dominate the **yellow** region of the spectrum. Due to their strong intensity and close proximity, these lines often appear as a single **bright-yellow** line when observed with standard laboratory equipment. (Figure 7.10)

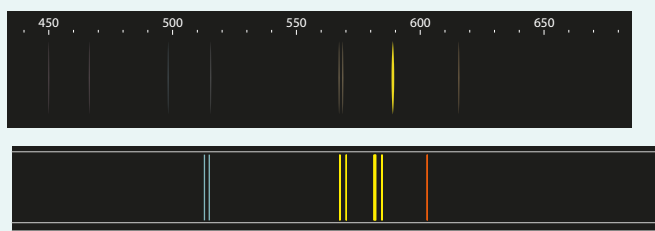


Figure 7.10

Strontium

Strontium's emission spectrum is dominated by strong **red** lines, particularly in the 640–670 nm range. Strontium also displays lines in the **blue** region, although these are less intense than the red. Some **orange** lines may also be present. The vibrant red glow produced by these lines makes it easy to recognise strontium, especially in flame tests. (Figure 7.11)

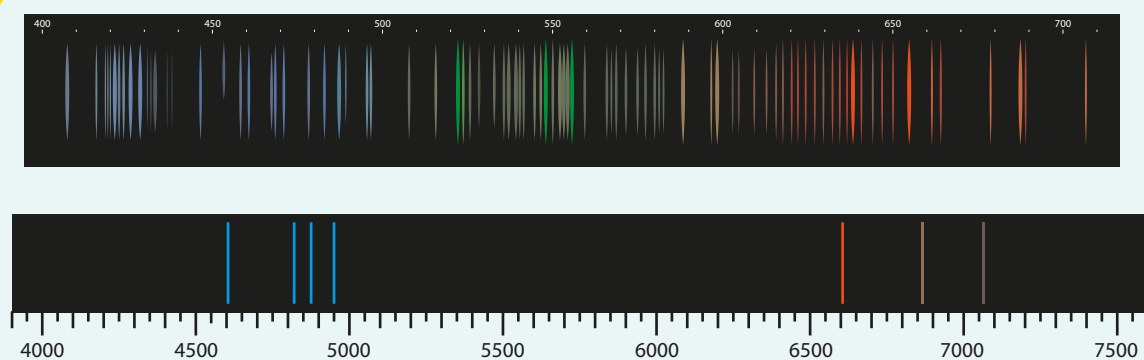


Figure 7.11

Copper

Copper's emission spectrum is characterised by distinct **blue-green** lines, notably around 510 nm and 521 nm. The **blue-green** glow produced by these lines makes copper easily recognisable, especially in flame tests, where, as we know, copper produces a distinctive **blue-green** flame. (Figure 7.12)

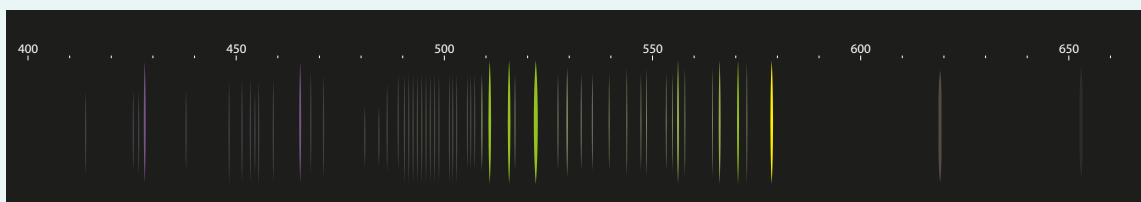


Figure 7.12

7.6 Sublevels

HL

As technology developed, scientists studying line emission spectra found **that what had originally seemed to be one line was actually a number of lines very close together**. These lines were too close together to have been produced by electrons transitioning between energy levels. **Scientists therefore reasoned that energy levels must be subdivided further – into sublevels – and that these lines must have been caused by electrons transitioning between sublevels.**

Scientists found that the first energy level has one sublevel, the second has two, the third has three, etc. There are four types of sublevel – named **s, p, d, f**. (They're named s, p, d and f after how their corresponding lines on emission spectra appeared – sharp, principal, diffuse and fundamental. You don't need to remember these names, only the letters.) An s sublevel has the lowest energy, with an increase in energy as we move to p, then d, with f being the highest energy sublevel. They're filled in order of increasing energy – e.g. in the fourth energy level ($n = 4$), the 4s sublevel is filled first, then 4p, then 4d, then 4f.



A **sublevel** is a subdivision of a main energy level (containing one or more atomic orbitals, all of which have the same energy).

Below is a breakdown of energy levels and their sublevels:

$n = 1$ 1s

$n = 2$ 2s 2p For example, the second energy level has two sublevels, 2s and 2p.

$n = 3$ 3s 3p 3d

$n = 4$ 4s 4p 4d 4f

Each type of sublevel can hold a specific number of electrons. **An s sublevel can hold two electrons, a p sublevel can hold six electrons, while a d sublevel can hold ten electrons** (an f sublevel can hold fourteen electrons, but you don't need to know how to fill f sublevels for the Leaving Certificate).

This fits with what you learnt in Junior Cycle. The first energy level ($n = 1$) has one sublevel (s), so we write it as 1s. If an s sublevel can hold two electrons, then the first energy level can hold two electrons. The second energy level has two sublevels – 2s and 2p – which can hold two and six electrons respectively, for a total of eight. This is the reason you learnt at Junior Cycle that the first energy level (you may have called them shells) of an atom could hold two electrons, and the second energy level could hold eight.

Energy level	Sublevel	Electrons
$n = 1$	1s	2 electrons
$n = 2$	2s 2p	8 electrons

7.7 Writing electronic configurations including sublevels

To write electronic configurations with sublevels, you must know three things:

1. The number of electrons in an atom of that element
2. The order in which sublevels are filled
3. The number of electrons each sublevel can hold

1. The number of electrons in an atom of that element

For this we simply look at the element on the periodic table. Since it's an atom, the number of protons will be equal to the number of electrons. Therefore, the atomic number of the element will tell us the number of electrons.

2. The order in which sublevels are filled

The **Aufbau** principle states that when building up the electron configuration of an atom in its ground state, the electrons occupy the lowest available energy levels.

The Aufbau (German for 'building up') principle tells us that sublevels are filled in order of increasing energy: 1s 2s 2p 3s 3p 4s 3d 4p 4d 4f. **It's important to note here that the 4s sublevel has less energy than the 3d sublevel.** 4s always fills before 3d. The best way to remember the order to fill sublevels is to write out the energy levels as seen in Figure 7.13 (1, 2, 3 and 4 vertically, listing all sublevels horizontally).

Once you have drawn that, draw arrows as shown in Figure 7.14.

Then simply follow the direction of the arrows to give you the filling order.

1s			
2s	2p		
3s	3p	3d	
4s	4p	4d	4f

Figure 7.13

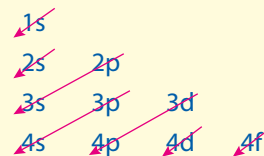


Figure 7.14

3. The number of electrons each sublevel can hold

As we know, an s sublevel can hold two electrons, a p sublevel can hold six electrons, a d sublevel can hold ten electrons (and an f sublevel can hold fourteen, but you don't need to know how to fill f sublevels for the Leaving Certificate).

Finally, to show how many electrons are in a specific sublevel, we add a superscript figure, as shown in figure 7.15.

If this were the full electronic configuration of the element, it would show helium, as it has only two electrons. This will all be easier to understand as you study the following examples.

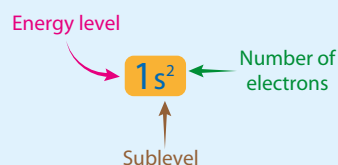


Figure 7.15

Example 3

Write out the electronic configuration of magnesium (including sublevels).

Magnesium
12
Mg
24.305

s = can hold 2 electrons
p = can hold 6 electrons
d = can hold 10 electrons
f = can hold 14 electrons

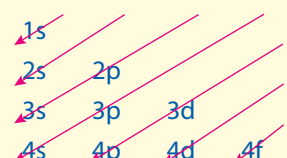


Figure 7.16

The atomic number of magnesium is 12. Following the filling order, the first sublevel to be occupied is 1s. An s orbital can hold two electrons, so the first thing we write is 1s². Next is 2s, which, again, can hold two electrons: 2s². Next to be filled is 2p, and we know that a p orbital can hold 6 electrons: 2p⁶. The last two electrons will go in the next sublevel to be filled: 3s².

Magnesium: 1s² 2s² 2p⁶ 3s²



Example 4

Write out the electronic configuration of calcium (including sublevels).

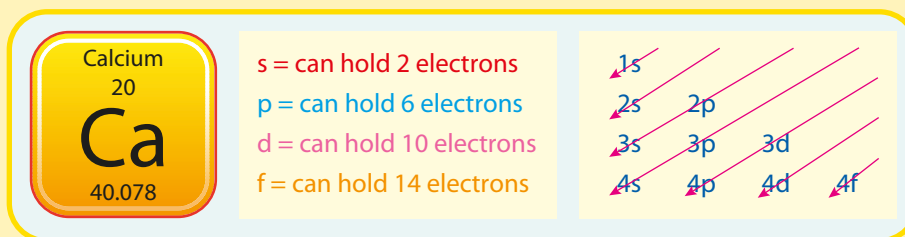


Figure 7.17

Calcium has twenty electrons. Again, we follow the filling order: 1s 2s 2p 3s 3p, etc., while remembering how many electrons each sublevel can hold.

Calcium: $1s^2 2s^2 2p^6 3s^2 3p^6 4s^2$



Test yourself!

- Which elements are the following electronic configurations showing?
 - $1s^2 2s^2 2p^4$
 - $1s^2 2s^2 2p^6$
 - $1s^2 2s^2 2p^6 3s^2$
 - $1s^2 2s^2 2p^6 3s^2 3p^6$
 - $1s^2 2s^2 2p^6 3s^2 3p^6 4s^2 3d^{10}$
- Write out the electronic configurations (include energy levels and sublevels) for: (a) Lithium; (b) Carbon; (c) Fluorine; (d) Aluminium; (e) Potassium

You are required to be able to do this for the first thirty-six elements of the periodic table. They are listed below.

Element	Atomic number	Electron configuration
Hydrogen (H)	1	$1s^1$
Helium (He)	2	$1s^2$
Lithium (Li)	3	$1s^2 2s^1$
Beryllium (Be)	4	$1s^2 2s^2$
Boron (B)	5	$1s^2 2s^2 2p^1$
Carbon (C)	6	$1s^2 2s^2 2p^2$
Nitrogen (N)	7	$1s^2 2s^2 2p^3$
Oxygen (O)	8	$1s^2 2s^2 2p^4$
Fluorine (F)	9	$1s^2 2s^2 2p^5$
Neon (Ne)	10	$1s^2 2s^2 2p^6$
Sodium (Na)	11	$1s^2 2s^2 2p^6 3s^1$
Magnesium (Mg)	12	$1s^2 2s^2 2p^6 3s^2$

Element	Atomic number	Electron configuration
Aluminium (Al)	13	$1s^2 2s^2 2p^6 3s^2 3p^1$
Silicon (Si)	14	$1s^2 2s^2 2p^6 3s^2 3p^2$
Phosphorus (P)	15	$1s^2 2s^2 2p^6 3s^2 3p^3$
Sulfur (S)	16	$1s^2 2s^2 2p^6 3s^2 3p^4$
Chlorine (Cl)	17	$1s^2 2s^2 2p^6 3s^2 3p^5$
Argon (Ar)	18	$1s^2 2s^2 2p^6 3s^2 3p^6$
Potassium (K)	19	$1s^2 2s^2 2p^6 3s^2 3p^6 4s^1$
Calcium (Ca)	20	$1s^2 2s^2 2p^6 3s^2 3p^6 4s^2$
Scandium (Sc)	21	$1s^2 2s^2 2p^6 3s^2 3p^6 4s^2 3d^1$
Titanium (Ti)	22	$1s^2 2s^2 2p^6 3s^2 3p^6 4s^2 3d^2$
Vanadium (V)	23	$1s^2 2s^2 2p^6 3s^2 3p^6 4s^2 3d^3$
Chromium (Cr)	24	$1s^2 2s^2 2p^6 3s^2 3p^6 4s^1 3d^5$
Manganese (Mn)	25	$1s^2 2s^2 2p^6 3s^2 3p^6 4s^2 3d^5$
Iron (Fe)	26	$1s^2 2s^2 2p^6 3s^2 3p^6 4s^2 3d^6$
Cobalt (Co)	27	$1s^2 2s^2 2p^6 3s^2 3p^6 4s^2 3d^7$
Nickel (Ni)	28	$1s^2 2s^2 2p^6 3s^2 3p^6 4s^2 3d^8$
Copper (Cu)	29	$1s^2 2s^2 2p^6 3s^2 3p^6 4s^1 3d^{10}$
Zinc (Zn)	30	$1s^2 2s^2 2p^6 3s^2 3p^6 4s^2 3d^{10}$
Gallium (Ga)	31	$1s^2 2s^2 2p^6 3s^2 3p^6 4s^2 3d^{10} 4p^1$
Germanium (Ge)	32	$1s^2 2s^2 2p^6 3s^2 3p^6 4s^2 3d^{10} 4p^2$
Arsenic (As)	33	$1s^2 2s^2 2p^6 3s^2 3p^6 4s^2 3d^{10} 4p^3$
Selenium (Se)	34	$1s^2 2s^2 2p^6 3s^2 3p^6 4s^2 3d^{10} 4p^4$
Bromine (Br)	35	$1s^2 2s^2 2p^6 3s^2 3p^6 4s^2 3d^{10} 4p^5$
Krypton (Kr)	36	$1s^2 2s^2 2p^6 3s^2 3p^6 4s^2 3d^{10} 4p^6$

Exceptions

It is very important to note that there are two exceptions to the regular filling order: copper and chromium. Note that chromium has an electronic configuration of $1s^2 2s^2 2p^6 3s^2 3p^6 4s^1 3d^5$, rather than $4s^2 3d^4$. Similarly, copper has an electronic configuration of $1s^2 2s^2 2p^6 3s^2 3p^6 4s^1 3d^{10}$ rather than $4s^2 3d^9$. This is because **half-filled or fully filled sublevels have extra stability**, so copper and chromium rearrange their electrons to achieve this.

7.8 Orbitals

You can now write electronic configurations showing energy levels and sublevels, but there is one last piece of the puzzle to complete. You also need to be able to write electronic configurations showing orbitals. As we know from Chapter 6:

An **orbital** is a region of space around the nucleus of an atom within which there is a high probability of finding an electron.



Sublevels contain orbitals. An orbital can hold two electrons. Therefore, an s sublevel contains one orbital, a p sublevel contains three, a d sublevel contains five (and an f sublevel contains seven).

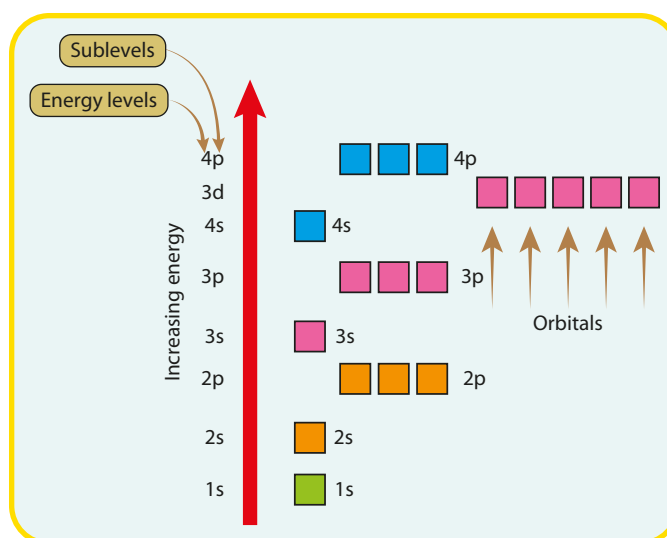


Figure 7.18

Pauli's exclusion principle states that no more than two electrons may occupy an orbital, and they must have opposite spin.

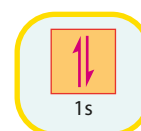


Figure 7.19

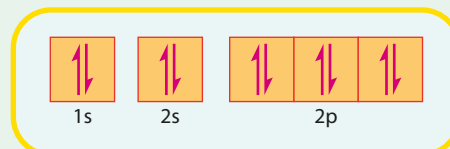
As we can see in Figure 7.18, 1s contains one orbital. 2s contains one orbital, while 2p contains three orbitals. We can depict electrons in orbitals as half-headed arrows. (see Figure 7.19).



Test yourself!

What element is depicted by the electronic arrangement shown in Figure 7.20?

Figure 7.20



Shapes of orbitals

As we learnt in Chapter 6, orbitals have shapes. An s orbital is spherical-shaped, while a p sublevel is composed of three dumb-bell shaped orbitals. These three p orbitals are named p_x , p_y , and p_z , and together make up a p sublevel – e.g. the 2p sublevel is composed of the orbitals $2p_x$, $2p_y$ and $2p_z$.

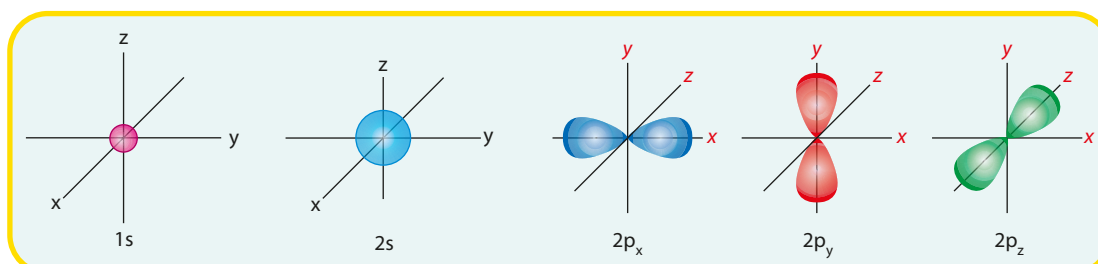


Figure 7.21

Energy level	Sublevels	No. of orbitals in each sublevel	Names of orbitals	No. of electrons each sublevel holds
$n = 1$	s	1	s	2
$n = 2$	s, p	1, 3	p_x, p_y, p_z	2, 6
$n = 3$	s, p, d	1, 3, 5	–	2, 6, 10
$n = 4$	s, p, d, f	1, 3, 5, 7	–	2, 6, 10, 14

You don't need to know the names for the d or f orbitals, so they are not included here.

Larger atoms have more than four energy levels, but since you must only know electronic configurations for the first 36 elements for the LC, we need not concern ourselves with those. However, you should be aware that they exist.

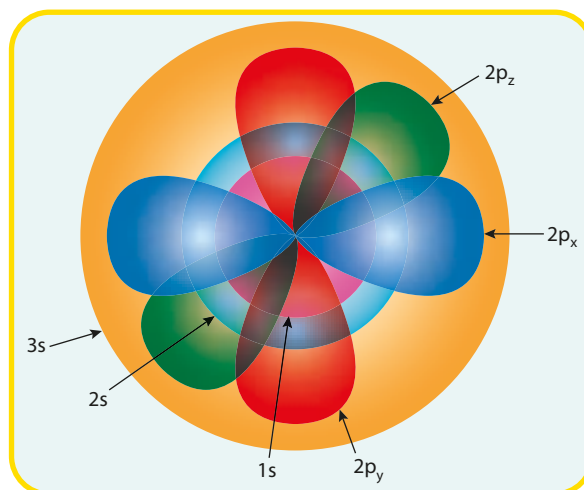


Figure 7.22



Crack It!

This analogy may help you. Energy levels are like the floors of a house, and sublevels are like the rooms on each floor. Different rooms have different number of bunkbeds (i.e. orbitals), each of which can accommodate two people (i.e. two electrons).

7.9 Final step: writing electronic configurations including orbitals

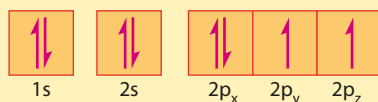
Since 1s and 2s have only one orbital, they remain the same. However, 2p must be broken down into its three orbitals: $2p_x, 2p_y, 2p_z$. To fill orbitals, we follow Hund's rule of maximum multiplicity.

Hund's rule of maximum multiplicity states that when two or more orbitals of equal energy are available, the electrons occupy them singly before filling them in pairs.

Example 5

Write the electronic configuration of oxygen, including sublevels.

Oxygen has eight electrons, which we have been writing as $1s^2 2s^2 2p^4$. However, to include sublevels we must now write this as $1s^2 2s^2 2p_x^2 2p_y^1 2p_z^1$.

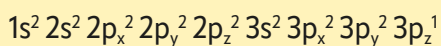




Example 6

State the number of (a) energy levels; (b) sub-levels; (c) orbitals occupied by electrons in a chlorine atom in its ground state.

To answer this question it's helpful to write out the electronic configuration of chlorine.



Now, we simply count.

(a) Energy levels = 1, 2, 3 = 3 energy levels

(b) Sublevels = 1s, 2s, 2p, 3s, 3p = 5 sublevels

(c) Orbitals = 1s 2s 2p_x 2p_y 2p_z 3s 3p_x 3p_y 3p_z = 9 orbitals



Test yourself!

Write **full** electronic configurations (*including orbitals*) for (a) fluorine; (b) aluminium; (c) calcium.

Writing electronic configurations of ions

Now that you are able to write the full electronic configurations of atoms, you can learn how to write the electronic configurations of ions.



Link it!

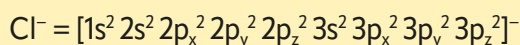
What is a cation? What is an anion? (See page ??)

Example 7

Write the full electronic configuration (showing energy levels, sublevels and orbitals) of Cl^- .

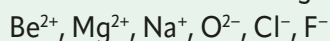
A chlorine atom has seventeen electrons. The minus sign tells us that Cl has gained an electron. Therefore, Cl^- has eighteen electrons. This gives us an electronic configuration of $1s^2 2s^2 2p_x^2 2p_y^2 2p_z^2 3s^2 3p_x^2 3p_y^2 3p_z^2$.

However, this could also be the electronic configuration of an atom with eighteen electrons – argon. Therefore, we can add square brackets and a charge to show it is an ion.

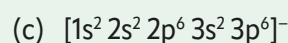
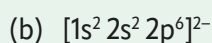
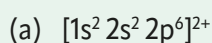


Test yourself!

1. Write the electron configuration of the following ions:



2. Determine the species represented by the following electronic configurations



For more questions on electronic configuration, see Chapter 7 in the accompanying skills book.

CHAPTER 9

Molecular Shapes and Intermolecular Forces (The perfect pair!)

Can I...



Use VSEPR theory to predict the shapes of molecules	
Visualise these molecules (draw diagrams, build 3D models, create digital models)	
Predict the overall polarity of a molecule when given its chemical formula	
Predict the overall polarity of a molecule when given a diagram	
Explain how molecules containing polar covalent bonds can be non-polar (i.e. link shape to overall polarity)	
Distinguish between intramolecular bonds and intermolecular forces	
Explain how permanent dipole-dipole forces arise	
Explain how hydrogen bonds arise	
Explain how London dispersion forces arise	
Explain how ion-dipole forces arise	
Explain how the type of intermolecular forces present can influence melting and boiling points (and therefore changes of state)	
Explain how the type of intermolecular forces present can influence solubility	
Interpret secondary data which provides evidence for the effects of intermolecular forces on melting and boiling points, and on solubility, accounting for trends	
Explain the effect of the shape and polarity of a molecule on its physical properties	
Explain the influence of polarity and symmetry on intermolecular forces, and therefore their influence on the properties of molecules	

Bold = HL only

9.1 VSEPR theory

We learnt in Chapter 8 that covalent compounds exist as molecules. Molecules contain different numbers of atoms, different types of bonds (e.g. polar or pure covalent) and exist in many different shapes. We use a theory called VSEPR (pronounced 'vesper') theory to predict the shape of a molecule. **VSEPR** stands for **valence-shell electron-pair repulsion** theory.

As we know, atoms share electrons to form molecules. The VSEPR theory is based on the fact that electron pairs in the valence shell (the outermost energy level) repel each other. **Since electron pairs repel each other, they'll arrange themselves as far away from each other as possible.** For instance, if a molecule has two

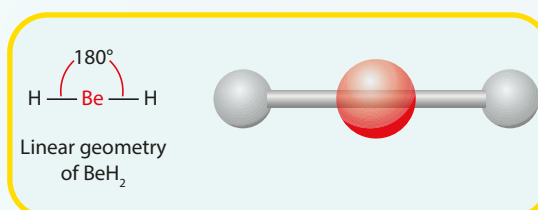


Figure 9.1

HL

electron pairs around its central atom, the electron pairs will position themselves as far apart as possible, resulting in a linear shape, with a bond angle of 180° (Figure 9.1). Note that the bond angle is the geometric angle between two neighbouring bonds (bonds that include a common atom).

However, it's not only the number of electron pairs that determines shape: it's also the type of electron pairs – i.e. are they bond pairs or lone pairs? When two electrons are **shared between atoms**, they're a **bond pair of electrons**. When two electrons aren't shared and aren't involved in a bond (i.e. belong to one atom only), they're a **lone pair of electrons**. Lone pairs have **extra repulsion power** – i.e. they repel other electron pairs to a greater extent than bond pairs do.

Since **lone pairs repel electron pairs to a greater extent, they'll change the shape of the molecule**. For example if one molecule has four bond pairs around the central atom and another molecule has three bond pairs and one lone pair, then the two molecules will be different shapes (even though both molecules have four electron pairs around the central atom).

Study the table below to see the various shapes that result depending on the combination of bond and lone pairs present around the central atom in a molecule.

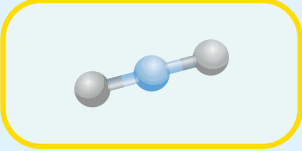
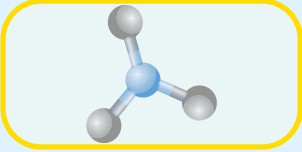
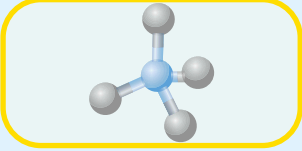
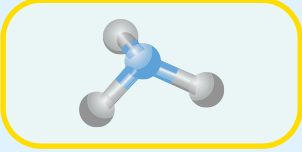
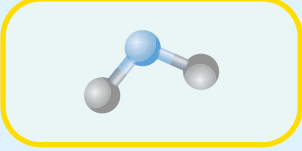
Total number of electron pairs around central atom	Number of bond pairs	Number of lone pairs	Shape of molecule	Diagrams	Bond angle
2	2	0	Linear		180°
3	3	0	Trigonal planar		120°
4	4	0	Tetrahedral		109.5°
4	3	1	Pyramidal		107°
4	2	2	V-shaped/ bent		104.5°

Table 9.1

The following examples will show you how to work out the shape of a molecule when given the molecular formula. For Leaving Certificate we can think of **the central atom in a molecule as the atom of which there is only one**.

**Example 1**

What shape is BeH_2 ?

Step 1: Count valence electrons of central atom

Be has four electrons, arranged 2,2. Therefore, it has two valence electrons.

Step 2: Add one electron for each bonding atom

There are two hydrogen atoms bonded to Be, so we add two: $2 + 2 = 4$

Step 3: Divide total by 2 to find the number of electron pairs

$$4 \div 2 = 2 \text{ pairs}$$

Step 4: Identify types of electron pairs and predict shape

Be is bonded to two hydrogen atoms – therefore, both pairs of electrons must be bond pairs. We saw in Table 9.1 (page ??) that a molecule with two bond pairs is **linear**, with a bond angle of 180° .

This makes sense when you remember that the VSEPR theory is based on electron-pair repulsion. Since each electron pair repels the other, the two electron pairs will arrange themselves around the beryllium atom in a way that keeps them as far away as possible from each other – hence, the 180° angle.

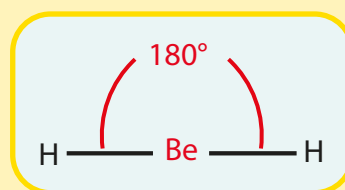


Figure 9.2

**Crack it!**

Step 1: Count valence electrons of central atom

Step 2: Add one electron for each bonding atom

Step 3: Divide total by 2 to find the number of electron pairs

Step 4: Identify types of electron pairs and predict shape. (Use Table 9.1, page ??). This table won't be provided in your exam – you must memorise it, including the bond angles)

Example 2

What shape is BCl_3 ?

Step 1: Count valence electrons of central atom

Boron has five electrons in total, arranged 2,3. Therefore, it has three valence electrons.

Step 2: Add one electron for each bonding atom

There are three chlorine atoms bonded to boron, so we add 3: $3 + 3 = 6$

Step 3: Divide total by two to find the number of electron pairs

$$6 \div 2 = 3 \text{ electron pairs}$$

HL

Step 4: Identify types of electron pairs and predict shape

B is bonded to three Cl atoms. Therefore, all three electron pairs are bond pairs.

We see in Table 9.1 (page ??) that a molecule with three bond pairs is **trigonal planar**, with a bond angle of **120°**.

Note that the three electron pairs will arrange themselves as far away as possible from each other – hence, the 120° bond angle.

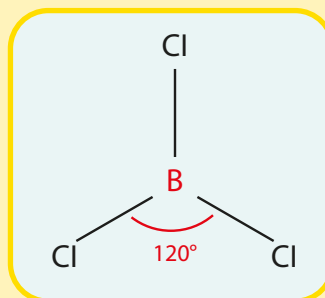


Figure 9.3

Example 3

What shape is CH₄?

Step 1: Count valence electrons of central atom

C has six electrons, arranged 2,4. Therefore, it has four valence electrons.

Step 2: Add one electron for each bonding atom

There are four hydrogen atoms bonded to carbon. Therefore, we add four: 4 + 4 = 8

Step 3: Divide total by 2 to find the number of electron pairs

$8 \div 2 = 4$ electron pairs

Step 4: Identify types of electron pairs and predict shape

The C atom is bonded to four H atoms. Therefore, all four electron pairs must be bond pairs. We saw in Table 9.1 (page ??) that a molecule with four bond pairs is **tetrahedral**, with a bond angle of **109.5°**.

It's very important to remember to draw the tetrahedral shape as shown as it's a 3-D molecule. The wedged line represents H coming out of the page towards you, and the dashed line represents H pointing away from you.

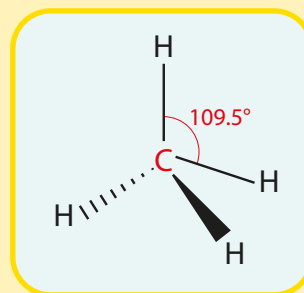


Figure 9.4



Try it!

Blow up four balloons to a similar size. Holding them at a central point, use them to demonstrate linear, trigonal planar and tetrahedral molecules.

Example 4

What shape is H₂O?

Step 1: Count valence electrons of central atom

O has eight electrons, arranged 2,6. Therefore, it has six valence electrons.

**Step 2:** Add one electron for each bonding atom

There are two hydrogen atoms bonded to oxygen, so we add two: $6 + 2 = 8$

Step 3: Divide total by 2 to find the number of electron pairs

$$8 \div 2 = 4 \text{ electron pairs}$$

Step 4: Identify types of electron pairs and predict shape

The O atom is bonded to two H atoms, so two of these electron pairs must be bond pairs.

Any remaining pairs are lone pairs. We saw in Table 9.1 (page ??) that a molecule with two bond pairs and two lone pairs is **V-shaped**. We draw H_2O in a V-shaped shape, with a bond angle of **104.5°** .

Note that although there are four electron pairs around the central atom (O), two are bond and two are lone pairs. Therefore, this will not be a tetrahedral shape, but a V-shaped molecule. The extra repulsion of the lone pairs pushes the bond pairs closer together, giving a bond angle of 104.5° , which is smaller than the bond angle in a tetrahedral shape – 109.5° .

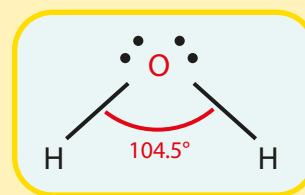


Figure 9.5

Example 5

What shape is NH_3 ?

Step 1: Count valence electrons of central atom

N has seven electrons, arranged 2,5. Therefore, it has five valence electrons.

Step 2: Add one electron for each bonding atom

There are three hydrogen atoms bonded to nitrogen, so we add three: $5 + 3 = 8$

Step 3: Divide total by 2 to find the number of electron pairs

$$8 \div 2 = 4 \text{ electron pairs}$$

Step 4: Identify types of electron pairs and predict shape

The N atom is bonded to three H atoms, so three electron pairs must be bond pairs, and therefore the remaining pair must be a lone pair. We saw in Table 9.1 (page ??) that a molecule with three bond pairs and one lone pair is **pyramidal**, with a bond angle of **107°** .

Note that since the lone pair has extra repulsion power, it pushes the three bond pairs further away from the lone pair than they are from each other.

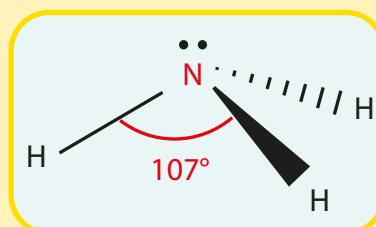


Figure 9.6



Crack it!

Molecules with a general formula AB_2 (i.e. one of one type of one atom – A – and two of another type of atom – B) will be either linear (e.g. BeH_2) or V-shaped (e.g. H_2O).

The two possible shapes for a molecule with general formula AB_3 are pyramidal (e.g. NH_3) or trigonal planar (e.g. BCl_3).

A molecule with a general formula AB_4 must be tetrahedral (e.g. CH_4).

9.2 Visualising molecules

Although we have already visualised molecules as 2-D diagrams, they are of course 3-D. To help you visualise the actual shapes of molecules, it's helpful to build models yourself, as well as looking at digital simulations.

3-D models

Molymod (molecular modelling) kits are often used by students in the lab to build models of molecules. Each colour in the kit refers to specific atoms. Your kit will come with instructions, but here's a guide to some of the most commonly used elements:

Carbon = black

Hydrogen = white

Oxygen = red

Nitrogen = blue

Halogen (group 17 element) = green



Figure 9.7



Try it!

Use a molymod kit to make models of the following molecules (you may need to use VSEPR theory first to work out their shape!): (a) CCl_4 (b) NH_3 (c) BF_3 .

Digital models

There are many different digital modelling programs available online (so feel free to explore!), but one good option is **molview.org**. Spend some time typing different compounds into the search bar and looking at the digital molecules generated. Compare these to your diagrams and to the 3-D models you made in the lab. What are the pros and cons of each type of model?

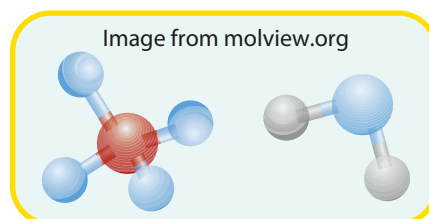


Figure 9.8



9.3 How shape affects polarity

Note: For OL, you must be able to determine how shape affects polarity (when given a diagram of a molecule), but not work out the shape of molecules. For HL, you must be able to do both.

At this point we have studied many molecules that contain polar covalent bonds. Now we must distinguish between a molecule containing polar covalent bonds and a polar molecule, since **not all molecules containing polar covalent bonds are polar molecules**.



Link it!

How can we determine if a covalent bond is polar or non-polar? (page ??)

Let's remind ourselves of what the word polar means. Polar indicates that a molecule has two poles of opposite charges. Electron density is focused at one end of the molecule, making it partially negative (δ^-) and leaving the other side partially positive (δ^+).

If a molecule has non-polar covalent bonds only, the molecule is also non-polar.

If a molecule has polar covalent bonds, it may be polar or non-polar.

A polar molecule must have two characteristics:

1. It must contain polar covalent bonds.
2. The centres of positive and negative charge must not coincide (the molecule must not be symmetrical).

Let's have a look at some examples to explain this.

Example 6: Water, H_2O

Determine if this molecule is polar or non-polar.

Step 1: Determine if the bonds are polar or non-polar covalent

The O-H bonds in a water molecule are polar covalent (electronegativity difference of 1.24).

Step 2: Determine if the centres of negative and positive charge coincide (if the molecule is symmetrical)

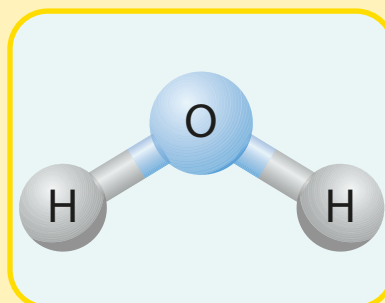


Figure 9.9

HL

Study Figure 9.10. We can see that the centre of partial negative charge in this water molecule is at the O atom. The centre of partial positive charge is midway between the hydrogen atoms. The centres of partial negative and partial positive charge aren't in the same place – they don't coincide. (If the centres of partially positive and partially negative charges coincide, they effectively 'cancel' each other out. Here, they don't.) The partial positive and partial negative poles are in different parts of the molecule – therefore, the molecule has two poles – i.e. is polar.

Another way of saying this is that the molecule is not symmetrical. If you fold this in half downwards on the dotted line, both sides of the molecule are not the same.

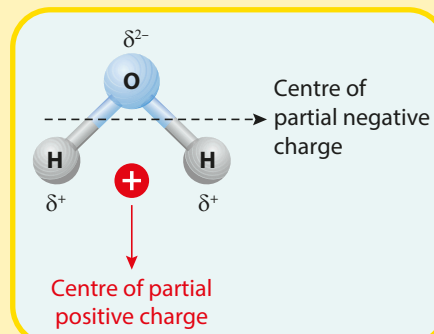


Figure 9.10

Example 7: Tetrachloromethane, CCl₄

Step 1: Determine if the bonds are polar or non-polar covalent

Let's look at a molecule of CCl₄. The C-Cl bonds are polar covalent (electronegativity difference of 0.61).

Step 2: Determine if the centres of negative and positive charges coincide (if the molecule is symmetrical)

Study Figure 9.12. We can see that the centre of positive charge is in the centre of the molecule – at the carbon atom. The centre of negative charge is also in the centre of the molecule – midway between all four chlorine atoms. The partial positive and partial negative poles of this molecule coincide and 'cancel' each other out. Therefore, this molecule is not a polar molecule.

Another way of saying this is that the molecule is symmetrical. Even if a symmetrical molecule contains polar bonds, the molecule will still be non-polar.

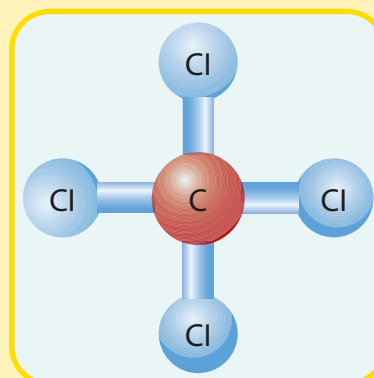


Figure 9.11

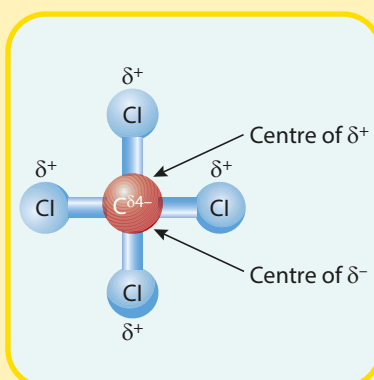


Figure 9.12

A molecule will be non-polar if:

1. It contains only non-polar covalent bonds.
2. It contains polar covalent bonds but the centres of negative and positive charge coincide (the molecule is symmetrical).



For OL students, you must link shape to polarity. Molecules containing polar covalent bonds that are linear, trigonal planar or tetrahedral will be non-polar (as long as the atoms surrounding the central atom are all the same). Molecules containing polar covalent bonds that are pyramidal or V-shaped will always be polar.



Test yourself!

Are the following molecules polar or non-polar?

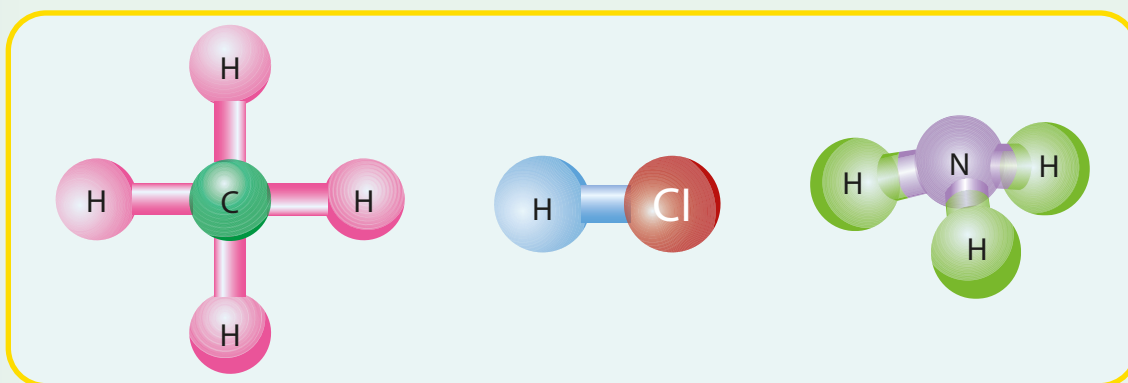


Figure 9.13

9.4 Intermolecular forces

We are now moving on from shapes to talk about intermolecular forces. As you should know from Chapter 8, intramolecular bonding refers to bonds inside a molecule (e.g. polar covalent bonds), **whereas intermolecular forces are the forces between molecules**. It's very important that this is very clear in your mind before you continue reading (studying Figure 9.14 will help you).

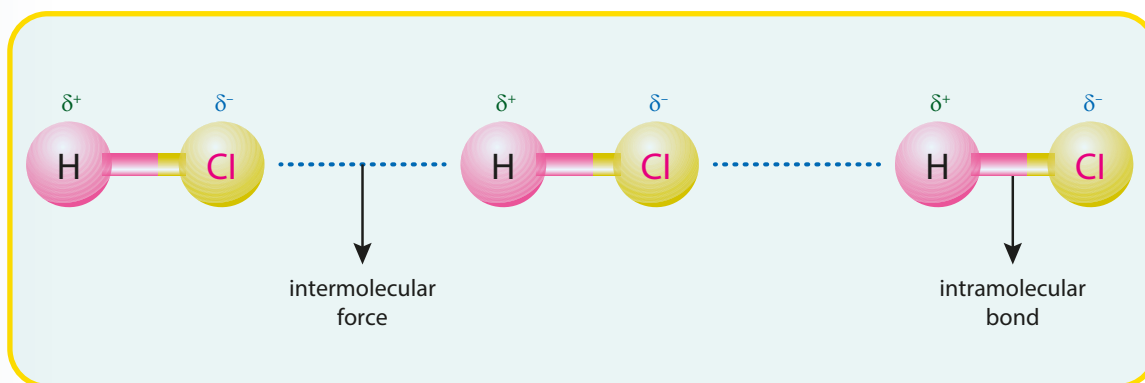


Figure 9.14

There are different types of intermolecular forces between molecules depending on the type of compound. The forces you will study are:

1. Permanent dipole-dipole forces (including hydrogen bonding)
2. London dispersion forces
3. Ion-dipole forces

1. Permanent dipole-dipole forces

Imagine a molecule of HCl. The intramolecular bond between the hydrogen atom and chlorine atom is covalent. As we have already learnt, this bond is polar covalent since the two electrons are not equally shared. Since the Cl atom is more electronegative (3.16), the shared pair of electrons is more attracted to it than to H (electronegativity = 2.20). This leaves the Cl atom slightly negative (δ^-) and the H atom slightly positive (δ^+). This separation of charge results in a **dipole** – i.e. there are two poles of charge in the molecule: one partially positive, one partially negative.

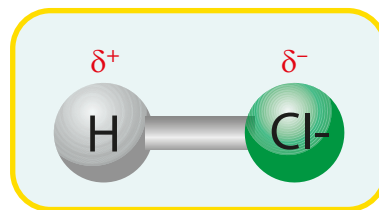


Figure 9.15

The slightly positively charged end of one molecule is attracted to the slightly negatively charged end of the other. This force of attraction between molecules is called a **permanent dipole-dipole force**.

Since the δ^+ and δ^- charged poles are permanent (due to electronegativity differences between the atoms), these intermolecular forces are also permanent.

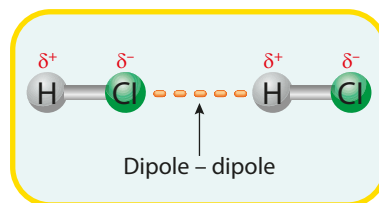


Figure 9.16

Permanent dipole-dipole forces exist between the negative pole of one polar molecule and the positive pole of another polar molecule.

Permanent dipole-dipole forces: hydrogen bonding

Hydrogen bonds are a special type of permanent dipole-dipole intermolecular force that occurs between **the hydrogen of one molecule and the nitrogen, oxygen or fluorine of another**.

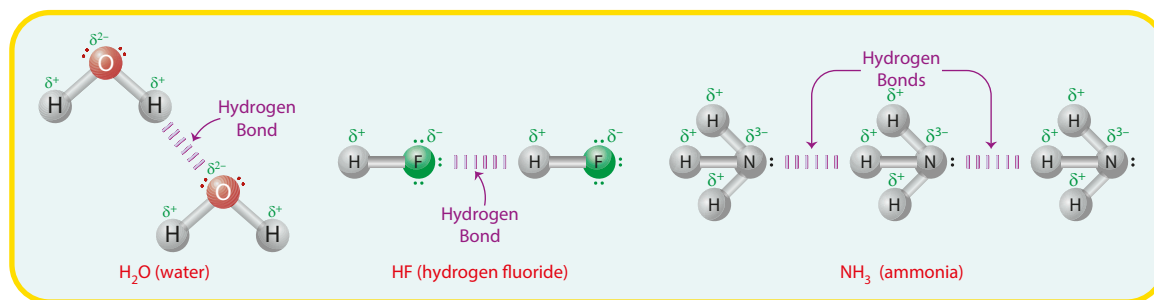


Figure 9.17

From the diagram you'll notice that this looks very similar to permanent dipole-dipole forces. However, atoms of nitrogen, oxygen and fluorine are all **very small and highly electronegative**. The large difference in electronegativity between **H and N, O or F** causes a **very strong dipole**. Essentially, hydrogen bonds are a **stronger type** of permanent dipole-dipole force.

Hydrogen bonds are a specific type of permanent dipole-dipole attraction between a hydrogen atom of one molecule and a small, highly electronegative atom (nitrogen, oxygen or fluorine) of a neighbouring molecule.



Note that for a **compound to have hydrogen bonding between its molecules** it must contain a hydrogen atom **directly bonded** to a nitrogen, oxygen or fluorine molecule. It's not just the presence of these atoms in a molecule – they must be **directly bonded to each other**.

(Don't be confused by the word 'bond' here: hydrogen bonds are still a type of intermolecular force.)

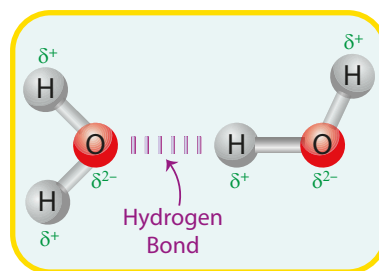


Figure 9.18

2. London dispersion forces

London dispersion forces are similar to permanent dipole-dipole forces except that they're **temporary**. They're named after Fritz London, who first explained this phenomenon. They're still a force of attraction between the partially positive end of a molecule and the partially negative end of a neighbouring molecule, except that those partial charges are very short-lived, and therefore the attraction between them is also short-lived.

So how do they occur?

Let's imagine a molecule of hydrogen. The intramolecular bond between the two hydrogen atoms is non-polar covalent, so electrons are shared equally between the two atoms (i.e. the two hydrogen atoms have an equal 'pull' over the shared pair of electrons in the covalent bond).

However, although it's true that neither atom is more electronegative than the other, at a specific moment in time both electrons can be closer to one end of the molecule than the other. This is because electrons are not fixed in position but instead move around (within orbitals, as we know from Chapters 6 and 7).



Link it!

What is an atomic orbital? What are the shapes of an s orbital and a p orbital? (page ??)

For this moment in time, one side of the molecule would be partially positive (δ^+) and the other partially negative (δ^-). When these temporary dipoles (δ^+ and δ^-) are set up, they can induce a dipole in a neighbouring hydrogen molecule.

Study Figure 9.19. Since one end of the H_2 molecule is slightly negative, it will repel the electrons in the neighbouring molecule (like repels like). This will cause the electrons in that molecule to shift, resulting in δ^+ and δ^- charges in that molecule also.

It's important to realise that **temporary** dipoles are set up, **not permanent** ones. Temporary dipoles don't last because electrons constantly move around at high speed, changing the partial charges in the molecule, so the attractions occur only for an instant. In fact, the next moment the molecules may look like Figure 9.20.

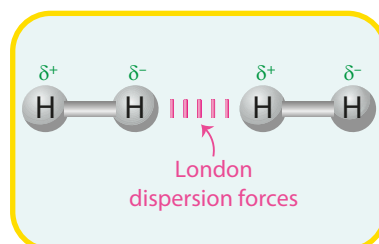


Figure 9.19

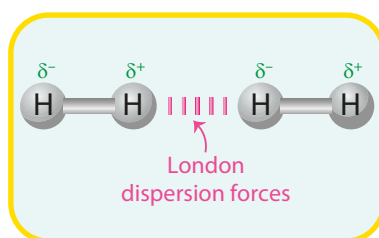


Figure 9.20

London dispersion forces are weak, temporary forces of attraction between neighbouring molecules as a result of temporary dipoles (caused by the movement of electrons within a molecule).

All molecules have London dispersion forces between them. For non-polar molecules – e.g. H_2 , O_2 , Cl_2 – they're the **only type of intermolecular forces** between molecules.

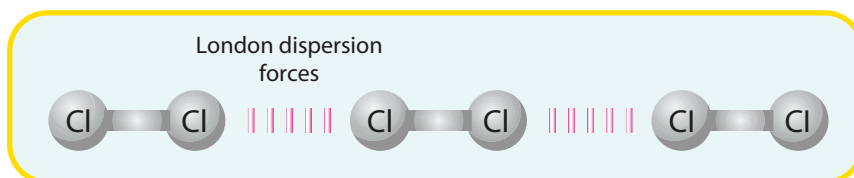


Figure 9.21

London dispersion forces are weaker than permanent dipole-dipole forces (when compared to comparable substances with the same or a similar number of electrons). This is because they're temporary.

3. Ion-dipole forces

Ion-dipole forces are forces of attraction between an ion and a molecule with a dipole.



Link it!

What is a cation? What is an anion? (See pages ?? and ??)

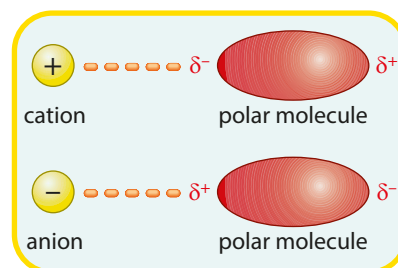


Figure 9.22

Opposites attract – cations will be attracted to the partially negative end of a polar molecule, while anions will be attracted to the partially positive end of a polar molecule (Figure 9.22). This force of attraction is an **ion-dipole force**.

Ion-dipole forces play a key role in dissolving ionic compounds in polar solvents – e.g. a solution of sodium chloride ($NaCl$) in water. (More on this on page ??.)

The strength of ion-dipole attractions depends on (1) the size of the charge on the ion; (2) the strength of the dipole on the molecule; (3) the distance between the ion and the dipole.

9.5 Intermolecular forces and physical properties: melting and boiling points

Intermolecular forces have a significant effect on physical properties, such as the melting or boiling point of the substance. This is because **attractive forces between molecules make molecules more difficult to separate**. Think of what we discussed in Chapter 3 – the process of melting and vaporisation. Particles must gain energy in order to change from a closely packed arrangement in a solid to the more widely spaced arrangement in a liquid (and they must gain even more energy to separate far apart enough to become a gas).



If the particles have strong attractive forces between them – i.e. **strong intermolecular forces** – then molecules must gain a significant amount of heat energy in order to weaken those forces and change state. This means the compound would have **high melting and boiling points**.

If the particles have weak intermolecular forces between them, a smaller amount of energy is required. Therefore, these substances would have lower melting and boiling points.

**Crack it!**

The stronger the intermolecular force, the higher the boiling point.

Two key factors affect the strength of intermolecular forces:

1. The type of intermolecular force
2. The molecular mass

1. Type of intermolecular force

Hydrogen bonds are the strongest. Permanent dipole-dipole forces are next in terms of strength. London dispersion forces are the weakest. (Also, remember that intermolecular forces are found between molecules of covalent compounds, but ionic compounds have the highest boiling points of all.)

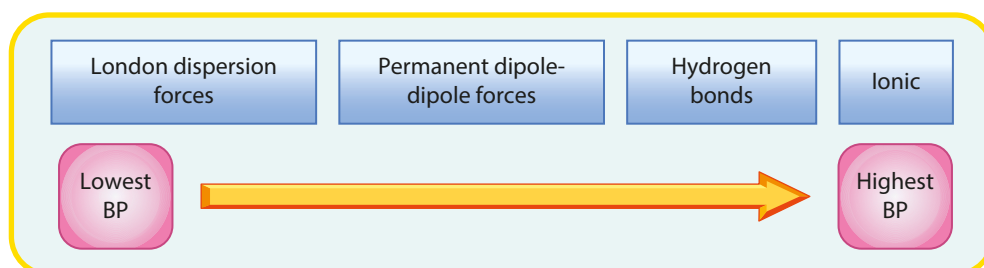


Figure 9.23

2. Molecular mass

The strength of intermolecular forces increases as the size of the molecule increases. This is because larger molecules have more electrons and can form stronger dipoles (dipoles with a greater imbalance of electrons). Stronger dipoles can induce stronger dipoles in neighbouring molecules. This increases the attraction between molecules – i.e. increases the strength of the intermolecular forces.

Example 8

List the following substances in order of increasing boiling point and justify your answer:
 H_2O , H_2 , HCl , O_2 .

List = H_2 , O_2 , HCl , H_2O

Justify = the stronger the intermolecular force (IMF) = the higher the boiling point.

The strongest IMF between molecules of H_2O is hydrogen bonds.

The strongest IMF between molecules of HCl is permanent dipole-dipole forces.

The strongest IMF between molecules of H_2 and O_2 is London dispersion forces.

Hydrogen bonds are stronger than permanent dipole-dipole forces and London dispersion forces, meaning that H_2O has the highest boiling point. Permanent dipole-dipole forces are stronger than London dispersion forces, meaning that HCl has the next highest boiling point.

Both H_2 and O_2 have only London dispersion forces between their molecules. However, oxygen has a larger molecular mass than hydrogen. This allows stronger temporary dipoles to form. This leads to stronger London dispersion forces between molecules of oxygen than between molecules of hydrogen. More energy is required to overcome stronger intermolecular forces and therefore oxygen has a higher boiling point.



Test yourself!

1. Ammonia (NH_3), nitrogen (N_2) and hydrogen chloride (HCl) have boiling points of -85.1°C , -33.34°C and -195.8°C . Which boiling point belongs to which compound? Justify your answer.
2. Study Table 9.2. Explain the trend in boiling points.

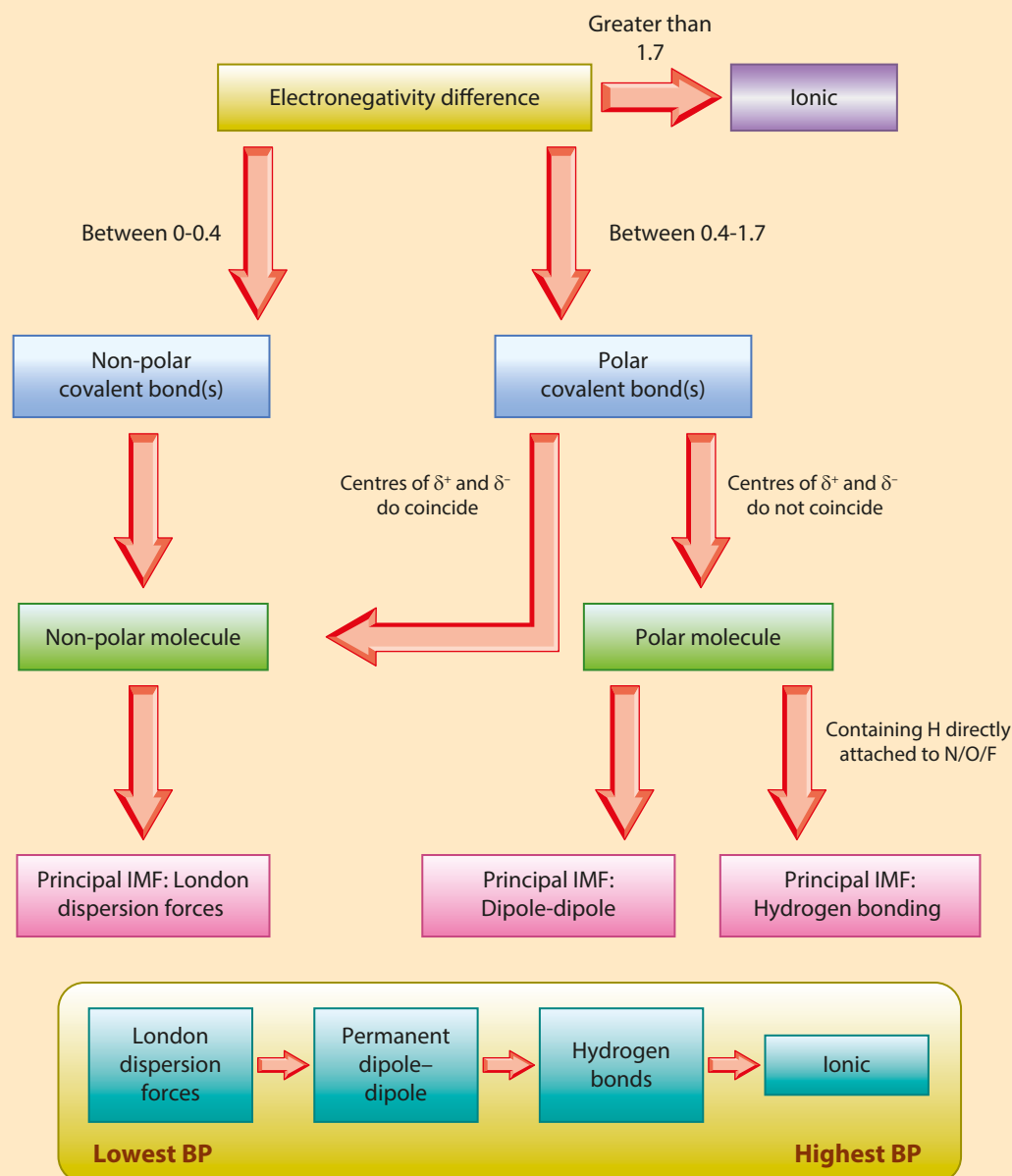
Compound	M_r	Boiling point ($^\circ\text{C}$)
Hydrogen, H_2	2.016	-252.9
Oxygen, O_2	32	-183
Chlorine, Cl_2	70.9	-34.04
Bromine, Br_2	159.8	58.8
Iodine, I_2	253.8	184.3

Table 9.2

HL



Crack it!



For any two compounds that have the same IMFs between their molecules, compare the size of the molecules (larger molecule = stronger IMF = higher BP).

9.6 Intermolecular forces and physical properties: solubility

In Chapter 8 we learnt that the golden rule for solubility is 'like dissolves like'. Now that we've studied intermolecular forces, we can explain why this is the case.

Polar solute in a polar solvent

Imagine using water (polar) as a solvent to dissolve ammonia (also polar). **The partial positive and negative charges on the water will be attracted to the partial positive and negative charges of the ammonia.** In fact, the attractions between the water (H_2O) and ammonia (NH_3) are hydrogen bonds. The water can surround the ammonia molecules and drag them apart – i.e. dissolve them.

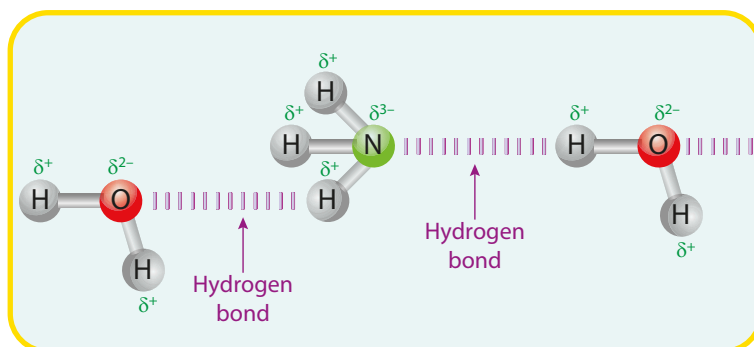


Figure 9.24

Ionic solute in a polar solvent

Ionic compounds like sodium chloride dissolve in polar solvents, e.g., salt in water, because the ionic bonding in NaCl is overcome by the **strong attraction between the ions and the polar water molecules – i.e. ion-dipole forces.**

The partially negative charges of the polar molecules attract positive ions (e.g. the $O^{\delta-}$ in H_2O attracts Na^+ in NaCl), while the partially positive charges of the polar molecules attract negative ions (e.g. the $H^{\delta+}$ in H_2O attracts Cl^- in NaCl).

It's these ion-dipole forces that allow the NaCl to dissolve – i.e. that allow ions to be dragged away from the crystal lattice and dispersed throughout the solution.

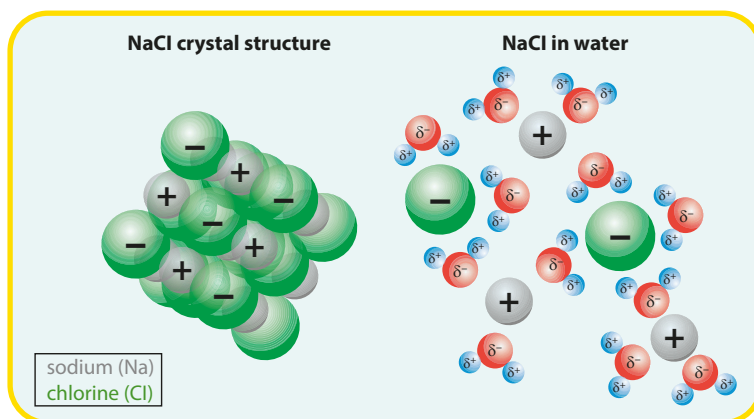


Figure 9.25

Non-polar solute in polar solvents

Non-polar substances have no charged ions or permanently partially charged molecules. Therefore, a polar solvent will not dissolve a non-polar solute – e.g. iodine crystals will not dissolve in water. This is because the water molecules will be more attracted to each other (they'll form hydrogen bonds with each other) than to the iodine. **The intermolecular forces between water molecules are stronger than those between water and iodine.**

Non-polar solute in non-polar solvent

A non-polar solvent will dissolve a non-polar solute because, **in the absence of stronger polar attractions, the non-polar solvent and solute will be attracted to each other by London dispersion forces.** Therefore, iodine crystals will dissolve in cyclohexane.



9.7 Effect of molecular shape on physical properties

The shape of its molecules determines some physical properties of the compound. For example, a molecule with intramolecular polar covalent bonds may be symmetrical – i.e. be a non-polar molecule. As a result it will have only London dispersion forces and have relatively low melting points and boiling points, as well as being insoluble in water.

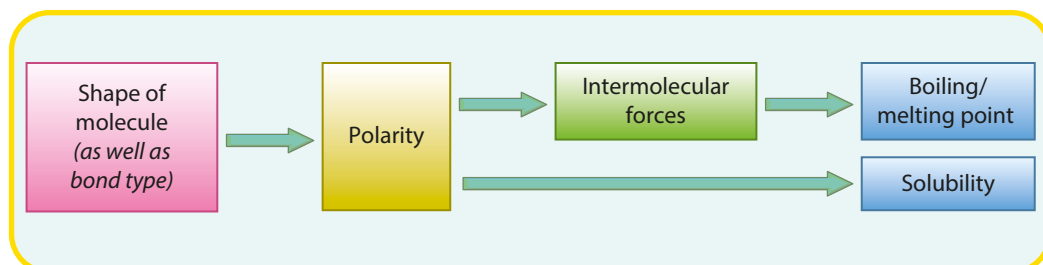


Figure 9.26



Test yourself!

1. Would you expect (a) methane (CH_4), (b) HCl to dissolve in water? Justify your answer.
2. Name a suitable solvent to dissolve hydrogen fluoride, HF.

For more questions on the molecular shapes and intermolecular forces, please see Chapter 9 in the workbook.

LEAVING CERTIFICATE CHEMISTRY

Features of the Student Textbook

Cracking Chemistry is a carefully constructed textbook that, in appropriate detail, prompts students to question, connect and integrate the various aspects of the new course. It will empower students to develop a scientific habit of mind and a secure understanding of the core concepts and fundamental principles of chemistry. Students will be able to apply these confidently to analyse and solve problems.

- Each chapter begins with a **student checklist** to guide learning and study. This is a clear list of what students must know and be able to do to fulfill the learning outcomes.
- All **definitions** are clearly highlighted (and a comprehensive list of all definitions will be available in the online resources).
- **Higher Level only content** is clearly marked throughout, making it easy to distinguish between Ordinary Level & Higher Level content.
- **Calculations:** All calculations are broken down into step-by-step instructions to aid student learning.
- **The AAC:** The book includes a student guide to the Chemistry in Practice (CIP) Investigation.

Student Portfolio Book

Students will complete **experiments, experimental investigations and research investigations** using the student portfolio. The student portfolio contains:

- All required experiments (including required chemicals & apparatus, step-by-step methods, risk assessments and questions to test knowledge and understanding).
- A structured approach to the experimental investigations (marked EI).
- A structured template for the four required research investigations.

Skills book

- This contains further questions and activities linked to each chapter in the textbook to enhance and reinforce learning.

Resources for Teachers

Comprehensive resources will be provided online for teachers, including:

- **The syllabus 'unpacked'** – a checklist for the entire specification.
- **A teacher guide to the AAC.**
- **Teacher material for each experiment** – how to prepare (a 'to do' list, along with instructions on making up required solutions), additional notes, answers to portfolio questions, etc.
- **Complete worked solutions** to all calculation questions (in both the workbook and textbook).
- **Class notes/student notes for each chapter** – condensed down to the essentials.
- **Stimulus material, activities and ideas for class.**

These resources will be regularly updated with extra materials (worksheets, tests, revision material, and more).

The author: Catherine Clayton is an experienced Science and Chemistry teacher, currently teaching at St Louis High School, Dublin. She completed her undergraduate degree at Trinity College Dublin and USCB (University of California Santa Barbara), followed by a Masters in Education at University College Dublin. Follow her on Instagram: @CrackingChemistry.