

POWERTRAIN & SUSTAINABILITY

Basics of Chemistry and Physics

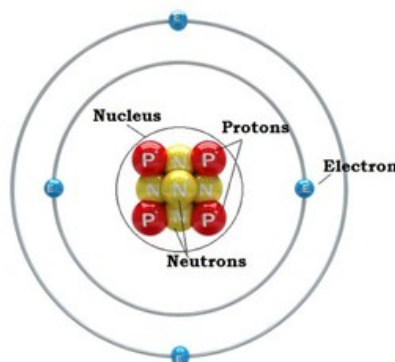
Dr Owen Williams – University of Wales TSD:

Atomic Structure and Periodic Table

Key Facts & Info:

- The particles constituting an atom are the **electron**, the **proton**, and the neutron.
- An **atom** is composed of two regions: the nucleus, which is in the centre of the atom and contains **protons** and neutrons, and the outer region of the atom, which holds its **electrons** in orbit around the nucleus.
- **Protons and neutrons** have approximately the same mass, about 1.67×10^{-27} kg, which scientists define as one atomic mass unit (Amu).
- Each **electron** has a negative charge (-1) equal to the positive charge of a proton (+1).
- Neutrons are uncharged particles found within the nucleus.
- The periodic table is a table that logically organize all the known elements.
- Each **row** is named “period” where all of the elements have the same number of atomic orbitals.
- Each column is called “**group**” where the elements have the same number of electrons in the outer **orbital**.

Every atom has a basic **nucleus** at the centre, consisting of a certain number of protons and neutrons. The number of this particles are different for different elements. Around the nucleus there is certain number of **electrons** in fixed orbits, at fixed energy levels.

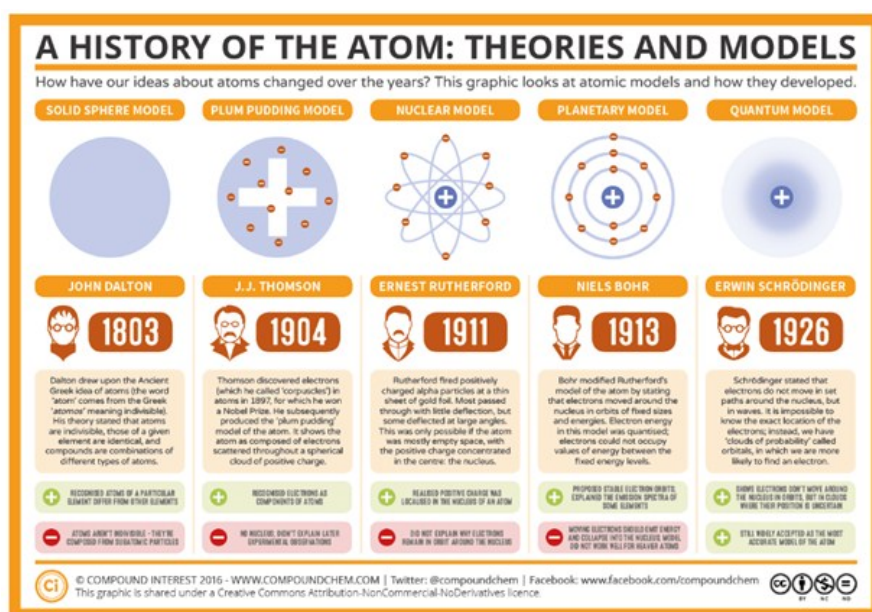


The electron is by far the smallest: At 9.11×10^{-31} kg and it carries a negative electrical charge. Usually, it is bound to the positively charged nucleus due to the attraction created from the opposite electric charges. If the electrons carried by an atom are more or fewer than its atomic number, then the atom becomes respectively negatively or positively charged. A charged atom is known as an **ion**.

Most of the **mass** of the atom comes from the protons and neutrons themselves, whereas electrons are almost 1/1837th times the weight of a proton or neutron. Protons and neutrons are both composed of other particles called quarks and gluons.

The **atomic number** is the number of protons (equal to the number of electrons in a neutral atom) in the atom and the **atomic mass number** is the sum of the number of protons and neutrons in the atom. The **atomic number** (Z) is defined as the number of units of positive charges (protons) in the nucleus. It is the number of protons in the nucleus that determines the chemical properties of an atom.

An atom may gain a positive or negative charge by either losing or gaining electrons respectively. Atoms may attach themselves to each other (of the same type or different type) to form molecules of different compounds, to form matter.



In some atoms, the nucleus can change naturally. Such an atom is **radioactive**. In nature, there are some elements that are radioactive, like uranium or radium. In labs, scientists can produce radioactivity by bombarding atoms with smaller particles.

The molecular mass of a substance is the sum of the atomic masses of all the atoms in a molecule of the substance. It is therefore the relative mass of molecule expressed in atomic mass units (u).

Isotopes are atoms in a chemical element having different numbers of neutrons than protons and electrons. The atoms in a particular element have the same number of protons and electrons but can carry varying numbers of neutrons.

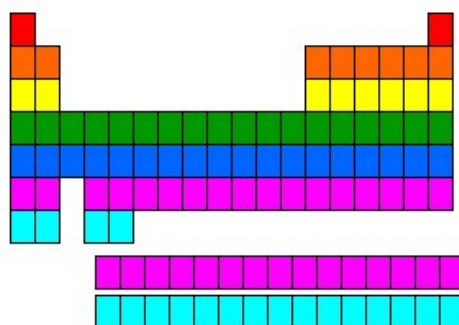
For example, **Hydrogen's** atomic number is 1, i.e. its nucleus contains 1 proton. It also has one electron. The Hydrogen atom is neutral since it contains the same number of protons and electrons (as the positive and negative charges cancel each other out).

However, approximately, one hydrogen atom out of 6000 contains a neutron in its nucleus. These atoms are still Hydrogen because they have one proton and one electron; they simply have a neutron that most hydrogen atoms do not carry. Hence, these atoms are called Isotopes.

There's also an isotope of hydrogen that contains two neutrons. It's called Tritium, it doesn't occur naturally on earth, but it can easily be created.

The Periodic Table

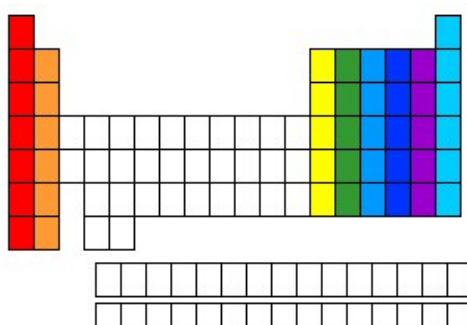
The **periodic table** is a table that logically organize all the known elements. Each **element** has a specific location according its atomic structure. Each row and column has specific characteristics.



A simplified periodic table diagram where each row is a different color. The colors from top to bottom are: red (1 row), orange (2 rows), yellow (2 rows), green (8 rows), blue (8 rows), magenta (8 rows), and cyan (2 rows). Below the main body, there are two additional rows: a magenta row and a cyan row.

PERIODS ALONG
HORIZONTAL ROWS

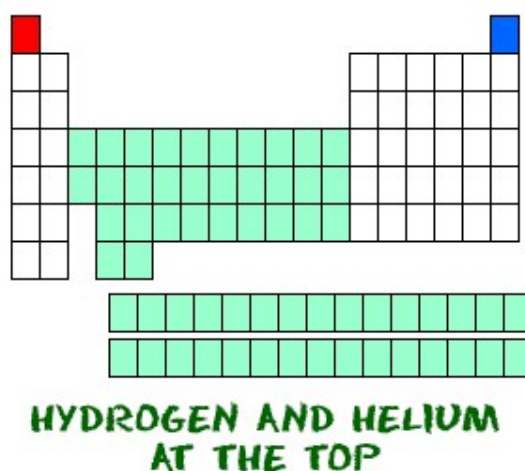
Each row is called a period where all of the elements have the same number of atomic orbitals. For example, every element in the top row (the first period) has one orbital for its electrons. All of the elements in the second row (the second period) have two orbitals for their electrons. As you move down the table, every row adds an orbital. At this time, there is a maximum of seven electron orbitals.



A simplified periodic table diagram where each column is a different color. The colors from left to right are: red (1 column), orange (2 columns), yellow (2 columns), green (1 column), blue (2 columns), purple (2 columns), and cyan (1 column). The rest of the table is white. Below the main body, there are two additional white rows.

GROUPS ALONG THE
VERTICAL COLUMNS

Each column is called a **group** where the elements have the same number of electrons in the outer **orbital**. Those outer electrons are also called **valence electrons**. They are the electrons involved in chemical bonds with other elements. Every element in the first column (group one) has one electron in its outer shell. Every element in the second column (group two) has two electrons in the outer shell.

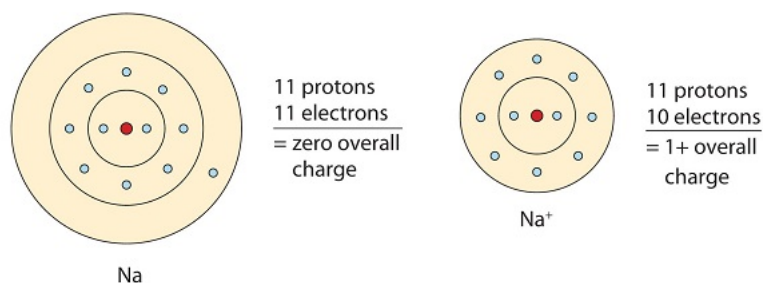


[Hydrogen](#) (H) and [helium](#) (He), in its neutral form, does not have a neutron. There is only one electron and one proton. Helium (He) is very stable with only two electrons in its outer orbital (valence shell). Even though it only has two electrons, it is still grouped with the noble gases that have eight electrons in their outermost orbitals, their valence shell is full.

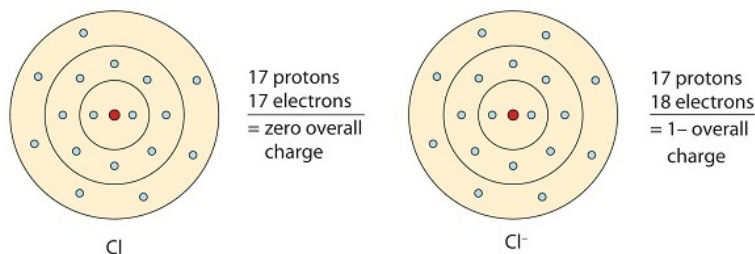
The periodic table can be used also to estimate some other properties of the atoms: electronegativity, ionization energy, electron affinity, atomic radius, melting point, and metallic character. You can use a [dynamic periodic table](#) tool to easily refer to specific elements and their atomic number, mass, orbital arrangement, etc.

There are many types of chemical bonds and forces that bind molecules together. The two most basic types of bonds are characterized as either ionic or covalent. In ionic bonding, atoms transfer electrons to each other. Ionic bonds require at least one electron donor and one electron acceptor. In contrast, atoms with the same electronegativity share electrons in covalent bonds, because neither atom preferentially attracts nor repels the shared electrons. Ionic bonding is the complete transfer of valence electron(s) between atoms. It is a type of chemical bond that generates two oppositely charged ions. In ionic bonds, the metal loses electrons to become a positively charged cation, whereas the nonmetal accepts those electrons to become a negatively charged anion. Ionic bonds require an electron donor, often a metal, and an electron acceptor, a non-metal.

Ionic bonding is observed because metals have few electrons in their outer-most orbitals. By losing those electrons, these metals can achieve noble gas configuration and satisfy the octet rule. Similarly, non-metals that have close to 8 electrons in their valence shells tend to readily accept electrons to achieve noble gas configuration. In ionic bonding, more than 1 electron can be donated or received to satisfy the octet rule. The charges on the anion and cation correspond to the number of electrons donated or received. In ionic bonds, the net charge of the compound must be zero.



This sodium molecule donates the lone electron in its valence orbital in order to achieve octet configuration. This creates a positively charged cation due to the loss of electron.



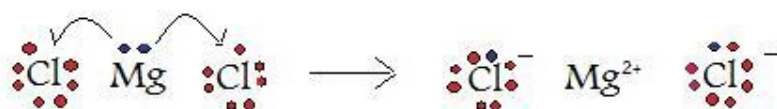
This chlorine atom receives one electron to achieve its octet configuration, which creates a negatively charged anion.

The predicted overall energy of the ionic bonding process, which includes the ionization energy of the metal and electron affinity of the non-metal, is usually positive, indicating that the reaction is endothermic and unfavourable. However, this reaction is highly favourable because of the electrostatic attraction between the particles. At the ideal interatomic distance, attraction between these particles releases enough energy to facilitate the reaction. Most ionic compounds tend to dissociate in polar solvents because they are often polar. This phenomenon is due to the opposite charges on each ion.

EXAMPLE 1: CHLORIDE SALTS (The salt you put on chips)



In this example, the sodium atom is donating its 1 valence electron to the chlorine atom. This creates a sodium cation and a chlorine anion. Notice that the net charge of the resulting compound is 0.



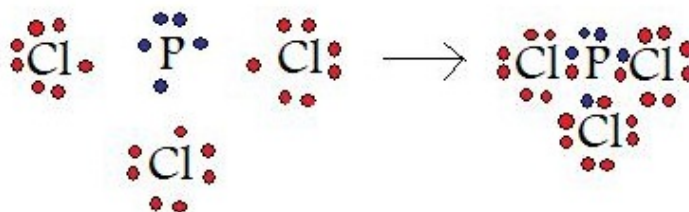
In this example, the magnesium atom is donating both of its valence electrons to chlorine atoms. Each chlorine atom can only accept 1 electron before it can achieve its noble gas configuration; therefore, 2 atoms of chlorine are required to accept the 2 electrons donated by the magnesium. Notice that the net charge of the compound is 0.

Covalent Bonding

Covalent bonding is the sharing of electrons between atoms. This type of bonding occurs between two atoms of the same element or of elements close to each other in the periodic table. This bonding occurs primarily between non-metals; however, it can also be observed between non-metals and metals.

If atoms have similar electronegativities (the same affinity for electrons), covalent bonds are most likely to occur. Because both atoms have the same affinity for electrons and neither has a tendency to donate them, they share electrons in order to achieve octet configuration and become more stable. In addition, the ionization energy of the atom is too large, and the electron affinity of the atom is too small for ionic bonding to occur. For example: carbon does not form ionic bonds because it has 4 valence electrons, half of an octet. To form ionic bonds, Carbon molecules must either gain or lose 4 electrons. This is highly unfavourable; therefore, carbon molecules share their 4 valence electrons through single, double, and triple bonds so that each atom can achieve noble gas configurations. Covalent bonds include interactions of the sigma and pi orbitals; therefore, covalent bonds lead to formation of single, double, triple, and quadruple bonds.

EXAMPLE 22: PCl_3Cl_3



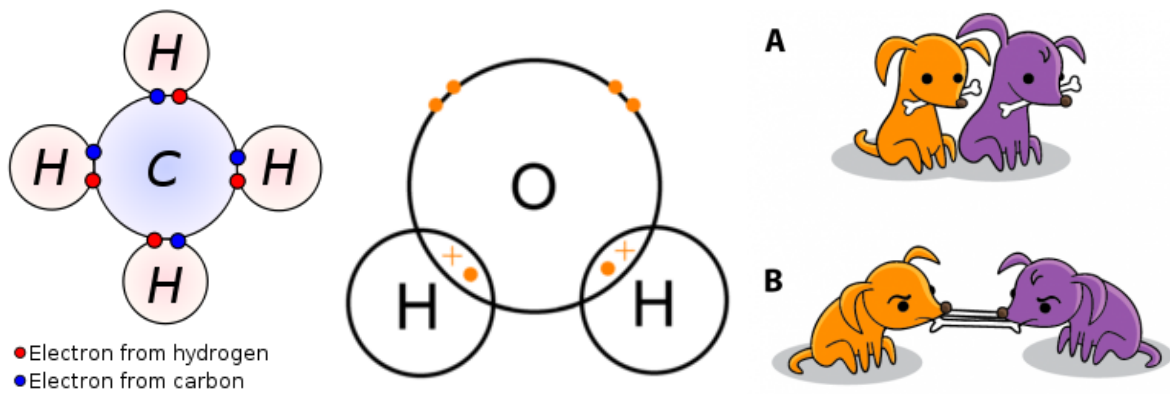
In this example, a phosphorous atom is sharing its three unpaired electrons with three chlorine atoms. In the end product, all four of these molecules have 8 valence electrons and satisfy the octet rule. This type of bonding will be very important as we look at fuels and combustion in later sessions.

Bonding in Organic Chemistry

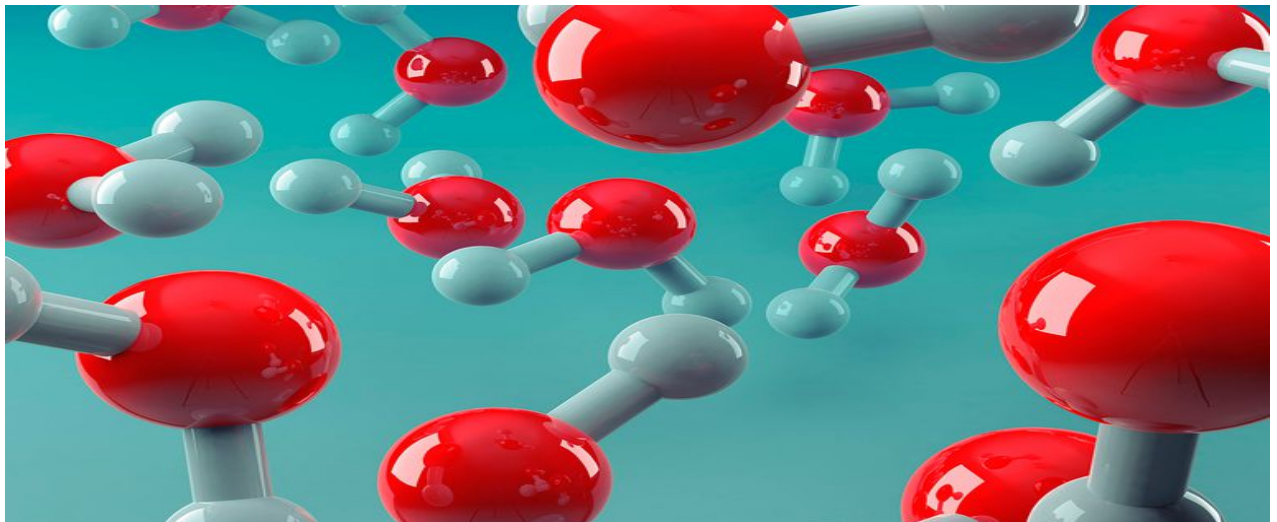
Ionic and covalent bonds are the two extremes of bonding. Polar covalent is the intermediate type of bonding between the two extremes. Some ionic bonds contain covalent characteristics and some covalent bonds are partially ionic. For example, most carbon-based compounds are covalently bonded but can also be partially ionic. Polarity is a measure of the separation of charge in a compound. A compound's polarity is dependent on the symmetry of the compound and on differences in electronegativity between atoms. Polarity occurs when the electron pushing elements, found on the left side of the periodic table, exchanges electrons with the electron pulling elements, on the right side of the table. This creates a spectrum of polarity, with ionic (polar) at one extreme, covalent (nonpolar) at another, and polar covalent in the middle.

Both of these bonds are important in organic chemistry. Ionic bonds are important because they allow the synthesis of specific organic compounds. Scientists can manipulate ionic properties and these interactions in order to form desired products. Covalent bonds are especially important since most carbon molecules interact primarily through covalent

bonding. Covalent bonding allows molecules to share electrons with other molecules, creating long chains of compounds and allowing more complexity in life.



(Methane CH_4 , Water H_2O , Dogs fighting over bones...)



Some Simple Organic Compounds

Dr Owen Williams – University of Wales TSD:

Approximately one-third of the compounds produced industrially are organic compounds. All living organisms are composed of organic compounds, as are most foods, medicines, clothing fibers, and plastics.

The simplest class of organic compounds is the hydrocarbons, which consist entirely of carbon and hydrogen. Petroleum and natural gas are complex, naturally occurring mixtures of many different hydrocarbons that furnish raw materials for the chemical industry. The four major classes of hydrocarbons are the following: the alkanes, which contain only carbon–hydrogen and carbon–carbon single bonds; the alkenes, which contain at least one carbon–carbon double bond; the alkynes, which contain at least one carbon–carbon triple bond; and the aromatic hydrocarbons, which usually contain rings of six carbon atoms that can be drawn with alternating single and double bonds.

Alkanes

The simplest alkane is methane (CH_4), a colorless, odorless gas that is the major component of natural gas. In larger alkanes whose carbon atoms are joined in an unbranched chain (*straight-chain alkanes*), each carbon atom is bonded to at most two other carbon atoms. The structures of two simple alkanes are shown in Figure 1, and the names and condensed structural formulas for the first 10 straight-chain alkanes are in Table 1. The names of all alkanes end in *-ane*, and their boiling points increase as the number of carbon atoms increases.

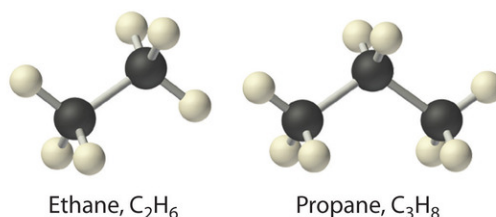


Figure 1 : Straight-Chain Alkanes with Two and Three Carbon Atoms

Alkanes with four or more carbon atoms can have more than one arrangement of atoms. The carbon atoms can form a single unbranched chain, or the primary chain of carbon atoms can have one or more shorter chains that form branches. For example, butane (C_4H_{10}) has two possible structures. *Normal* butane (usually called *n*-butane) is $\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_3$, in which the carbon atoms form a single unbranched chain. In contrast, the condensed structural formula for *isobutane* is $(\text{CH}_3)_2\text{CHCH}_3$, in which the primary chain of three carbon atoms has a one-carbon chain branching at the central carbon. Three-dimensional representations of both structures are as follows:

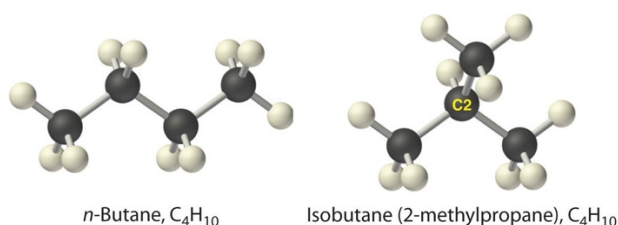


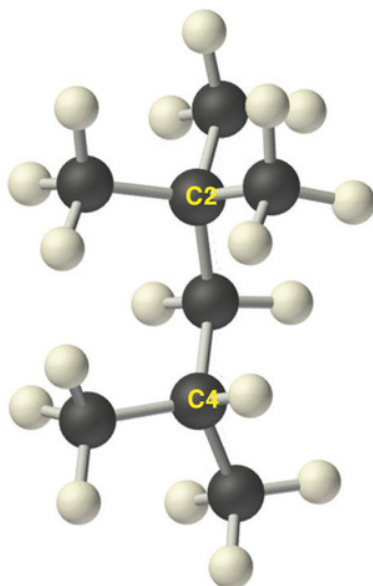
Table 1: The First 10 Straight-Chain Alkanes

Name	Number of Carbon Atoms	Molecular Formula	Condensed Structural Formula	Boiling Point (°C)	Uses
methane	1	CH ₄	CH ₄	-162	natural gas constituent
ethane	2	C ₂ H ₆	CH ₃ CH ₃	-89	natural gas constituent
propane	3	C ₃ H ₈	CH ₃ CH ₂ CH ₃	-42	bottled gas
butane	4	C ₄ H ₁₀	CH ₃ CH ₂ CH ₂ CH ₃ or CH ₃ (CH ₂) ₂ CH ₃	0	lighters, bottled gas
pentane	5	C ₅ H ₁₂	CH ₃ (CH ₂) ₃ CH ₃	36	solvent, gasoline
hexane	6	C ₆ H ₁₄	CH ₃ (CH ₂) ₄ CH ₃	69	solvent, gasoline
heptane	7	C ₇ H ₁₆	CH ₃ (CH ₂) ₅ CH ₃	98	solvent, gasoline
octane	8	C ₈ H ₁₈	CH ₃ (CH ₂) ₆ CH ₃	126	gasoline
nonane	9	C ₉ H ₂₀	CH ₃ (CH ₂) ₇ CH ₃	151	gasoline
decane	10	C ₁₀ H ₂₂	CH ₃ (CH ₂) ₈ CH ₃	174	kerosene

The systematic names for branched hydrocarbons use the lowest possible number to indicate the position of the branch along the longest straight carbon chain in the structure. Thus, the systematic name for isobutane is 2-methylpropane (see diagrams above), which indicates that a methyl group (which is a branch consisting of CH₃) is attached to the second carbon of a propane molecule.

Automotive Petrol

Similarly to isobutane described above, one of the major components of pump fuel (Petrol/Gasoline) is commonly called **isooctane**; its structure is as follows:



Isooctane (2,2,4-trimethylpentane)

The compound has a chain of five carbon atoms, so it is a derivative of pentane. There are two methyl group branches at one carbon atom and one methyl group at another. Using the lowest possible numbers for the branches gives 2,2,4-trimethylpentane for the systematic name of this compound.

It is still however C_8H_{18} 😊

Notice that there are a number of different compounds and structures labelled as 'Gasoline'. This is normal since the true chemical composition can be a complex mix of different things and varying molecular structures depending on the 'type' of petrol, the manufacturer and the country of origin. This is some pretty interesting stuff and makes things a little more complicated.

The Chemistry of Diesel Fuel

Dr Owen Williams – University of Wales TSD:



Diesel fuel is a liquid fuel that is made from the by-product of petroleum. Diesel fuel was originally supposed to be coal dust, but in 1895, Rudolf Diesel discovered the use of petroleum by-products for liquid fuel in diesel engines. The military likes using diesel because it is less flammable and is less prone to stalling unlike gasoline engines. Diesels are also more capable of producing higher torque than gasoline engines... (why?)

Composition of ...

- Crude Oil
 - Hydrocarbons (hydrogen and oxygen)
 - Paraffins (roughly 75%)
 - Carbon atoms that link, forming chain like molecules.
 - N-paraffins
 - Iso-paraffins
 - **Ranging from $C_{10}H_{22}$ to $C_{20}H_{42}$**
 - Aromatics (roughly 25%)
 - Similar to Naphthene, a ring like structure is created, but they are joined by aromatic (double) bonds, instead of single bonds.
 - **$C_{10}H_8$ - $C_{20}H_{34}$**
- Sulphur
- Nitrogen

Main Chemicals, Compounds, Components

Paraffins

There are two kinds of paraffins: N (normal) paraffins and Isoparaffins. N-paraffins have carbon atoms that will form chain-like molecules. Isoparaffins are similar to N-paraffins except they have offshoots or branches of carbons from the chain. It was first commercially produced in 1867, paraffin wax is known for its colorless, or white appearance when solid; however when it is a liquid it turns mostly translucent. It's melting point ranges from 50 to 65°C. However, there isn't just one type of paraffin wax, common types of paraffins in diesel fuel are: decane, n-pentadecane, methyltetradecane, eicosane, and methylnonadecane. Because paraffins have a straight molecular structure, paraffins are the main reason why diesel fuel will eventually begin to turn into a solid state, a process known as gelling, a big problem for diesel engines. At 0°C the paraffin in the fuel will begin to cloud the fuel, and at -12°C it will begin to "gel" and make a diesel engine unable to run. Kerosene can be added to the fuel beforehand, reducing the fuel's viscosity and making it much less prone to gelling.

Aromatics

Aromatics create a ring like structure with some of their carbon atoms. Aromatic hydrocarbon rings are created with 6 carbon atoms. They alternate single and double bonds throughout their ring structure. Another type of aromatic hydrocarbon is a polycyclic aromatic. Polycyclic aromatics are simply put as aromatic compounds with two or more aromatic rings. The simplest of all the aromatic compounds is benzene, with a chemical composition of C_6H_6 . The

name comes from the fact that the compounds of aromatics have a very strong aroma. Aromatic compounds are used to thin out oil or grease-based compounds, which explains why when kerosene and other compounds can be added to diesel fuel to change the diesel fuel's viscosity, making it less prone to gel up. Common compounds found in diesel fuel are naphthalene, tetralin, anthracene, and tetradecyl benzene.

Chemistry's Role

None of the components in diesel fuel are individually made. Diesel fuel could be seen as something that naturally occurs as it is extracted from the earth (oil), but the final product, diesel fuel, is a man-made product. The crude oil that is extracted from the earth is put in a distillation tower; the oil is then heated up to over 400°C. This begins a process, known as separation, that separates different components that have different boiling temperatures. As you go up the distillation tower the boiling temperature is cooler, and the refining process is more tedious. Diesel fuel is created at the lower end of the tower, then comes kerosene, gasoline, butane, and propane. These compounds are then collected by a distillation plate, which takes that compound away and stores it in a storage tank. Chemistry plays a big role in this process, as scientists need to know the chemical composition of each mixture (ex. how many hydrogen and carbon atoms are in each compound) that is being separated at each boiling point. They need to know where to put the distillation plates in the tower to collect each compound effectively and efficiently.

Interestingly, Petrol and Diesel are produced in roughly the same quantities are a part of the distillation process... and you can't really make the one without the other.... We may have a lot of unused diesel soon!

