Sustainability Profile: Simple Substances

In 1987 physical chemist P. W. Atkins published a beautiful book entitled *Molecules* that was part of the Scientific American Library collection. A Second Edition was published in 2003. This volume should be on the bookshelf (and maybe even the coffee table) of every chemist. After a brief introduction on some of the basics of chemistry, Atkins goes through 160 important molecules, shows the structure and describes the importance in one or two pages for each one. He starts with the elements and compounds found in air include modern air pollutants. He then moves to water, ammonia, methane (the main component of natural gas), and then simple organic compounds like alcohol, acetic acid (vinegar), formaldehyde, acetaldehyde. This book is the inspiration for this first Sustainability Profile where we introduce some of the most abundant substances that make up our environment and some lesser abundant substances, usually introduced by human activity, that degrade that environment.

Through these elements and compounds we will introduce several principles of General Chemistry: classification of matter, naming chemical substances, chemical structure and three dimensional shape. We will use these molecules as examples when we talk about these various topics, so refer back to this Sustainability Profile throughout the course. We will introduce these molecules in the context of the topic of classification of matter. We will mention other aspects (nomenclature, structure, shape), but will cover the chemical concept later in the course. Our discussion of each will include a brief mention of why these molecules are important from an environmental and sustainability perspective. For now we want you to see these substances as elements and compounds and to understand the importance of these molecules from that perspective.

AIR

Air is a mixture of gases that make up the earth's atmosphere. Dry air (with no water vapor present) is 78% nitrogen gas (N_2), 21% oxygen gas (O_2), 0.9% argon gas (Ar). There are other trace substances, most notably carbon dioxide (CO_2) at 0.0415% (more commonly written as 415 parts per million (ppm)) and pollutants such as carbon monoxide (CO); SO_2 and SO_3 (collectively known as SO_x); NO, NO_2 and N_2O (collectively known as NO_x); ozone (O_3); and hydroxyl radical (OH•). You can begin to see the importance of oxygen in general—many of these trace compounds are oxides, compounds of oxygen.

Nitrogen is an element (a pure substance made of only one kind of atom). In the atmosphere and in its most common form nitrogen is diatomic, N_2. It is a non-reactive molecule that makes up 78% of the earth's atmosphere. The Lewis structure of N_2 is $:N\equiv N:$ with a triple bond and a lone pair on each nitrogen. Each nitrogen atom contributes 5 electrons and shares 3 with the other nitrogen atom in the triple bond. Nitrogen is one of the four most common elements in living systems, but N_2 is not the direct source—it is too non-reactive. N_2 must be "fixed" by microorganisms (some associated with legume roots) or by chemical methods (the Haber process) in the form of ammonia/ammonium (NH_3/NH_4^+), nitrates (NO_3^-), or urea $NH_2(C{=}O)NH_2$. Pure nitrogen is produced by liquifying air and separating the nitrogen from the other components of air by distillation.

Oxygen is an element. In the atmosphere and in its most common form oxygen is diatomic, O_2. A less common form of oxygen (a different allotrope) is ozone, O_3 (discussed later). Oxygen is very reactive molecule that makes up 21% of the earth's atmosphere. The Lewis structure of O_2 is $:\ddot{O}{=}\ddot{O}:$ with a double bond and two lone pairs on each oxygen. Each nitrogen atoms contributes 6 electrons and shares 2 with the other oxygen atom in the double bond. Many substances on earth (molecular and ionic) are oxides due to this reactivity. A combustion reaction is a reaction of a substance (often a fuel) with oxygen to produced a violent reaction that gives off heat and light. On earth oxygen is primarily produced by photosynthetic plants. Oxygen is required by aerobic organisms in cellular respiration. In cellular respiration and in combustion reactions involving carbon compounds oxygen is released in the form of carbon dioxide, CO_2 and water, H_2O. Pure oxygen is also produced by liquifying air and separating it from the other components of air by distillation.

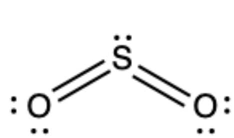
reactive since it has the full number of 8 outer shell electrons. Pure argon is also obtained by liquifying air and separating it from other components by distillation. Argon is used where inert (especially oxygen-free) atmospheres are needed. Argon can also be used in lighting where argon atoms emit light after being excited.

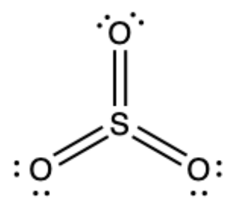
Water, H_2O, is a compound (a pure substance made of two or more kinds of atoms). It is also present in the atmosphere as water vapor (between 0-4%). We experience it as humidity. The amount of water that can be in the atmosphere is dependent on temperature. Relative humidity is the percent of water vapor out of the maximum possible at a given temperature. The percentages given above for the composition of the atmosphere do not include water—they are the composition of dry air. Clouds and fog are small droplets of water (aerosols) that have condensed from water vapor but that remain suspend in the air due to how small they are. Water is greenhouse gas, molecules that absorb infrared (IR) light and cause the warming of the atmosphere—more on greenhouse gases later as well. We will discuss liquid water in more detail below.

Carbon dioxide, CO_2, is a compound. It makes up about 0.04% of the atmosphere (also measured in parts per million (ppm)—100% = 1,000,000 ppm). CO_2 is a molecular compound (vs. an ionic compound) and is named using molecular binary (two different kinds of atoms) compound naming rules where prefixes (mono, di, tri, etc.) are used to tell how many of each atom is present—so one carbon and two oxygens would give monocarbon dioxide. The mono prefix is left off if it is on the first element, so the actual name is carbon dioxide. The concentrations of CO_2 are increasing due to the combustion of carbon containing materials such as coal, oil, and natural gas. At the beginning of the industrial revolution the CO_2 concentration was 280 ppm; this year we surpassed 420 ppm. This is a record high in the history of the human species. CO_2 comes from outgassing of volcanoes by heating carbonate (CO_3^{2-}) minerals (and cement production where $CaCO_3$ is heated to give CaO (a component of cement) and CO_2, combustion of carbon containing materials in forest and grass fires and fossil fuel combustion, and cellular respiration by biological organisms. The Lewis structure of CO_2 is $:\ddot{O}=C=\ddot{O}:$ and the molecule has a linear structure, i.e. the three atoms are in a straight line with a 180° bond angle. CO_2 is the most important greenhouse gas because of its presence due to human burning of fossil fuels. CO2 is non-reactive; more or less is it completely reacted (oxidized) carbon.

Carbon monoxide, CO, is a compound that is considered a pollutant caused by the incomplete combustion of carbon containing materials (fossil fuels and biological materials burned in fires). The catalytic converter in a car exhaust converts CO to CO_2. CO is a molecular compounds and so gets its name from there being one carbon and one oxygen (the prefix mono- is not sure with the first carbon). The Lewis structure of CO is $:C\equiv O:$ with a CO triple bond and one lone pair on the carbon and one lone pair on the oxygen. Notice that CO is an exception to the pattern that carbon normally makes 4 bonds and oxygen normally makes 2. CO is toxic and even lethal to humans. It binds to hemoglobin very tightly the way oxygen binds, but it is never released, preventing oxygen transport from the lungs.

Sulfur dioxide, SO_2, and **sulfur trioxide**, SO_3, are gaseous molecular compounds that are pollutants formed by the combustion of fuels that contain sulfur and the smelting of sulfur containing minerals. Binary molecular naming rules apply, hence the use of the prefixes di- and tri-; again, the prefix mono- might be expected, but it is not used if the single sulfur is the first element in the name. The Lewis structures are shown below. In SO_2 there are 2 double bonds from the central S atom to the 2 O atoms and a lone pair on the central S atom. In SO_3 there are 3 double bonds from the central S atom to the 3 O atoms. These structures are exceptions to the octet rule, 10 electrons around the central S atom in SO2 and 12 electrons around the central S atom in SO3. We say that S has an expanded octet. Sulfur is in Period 3 of the Periodic Table where *d* orbitals are available for bonding. This allows for more than 8 bonding and non-bonding electrons.

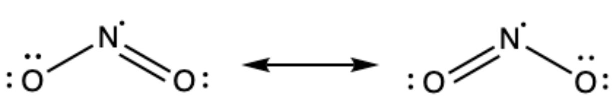


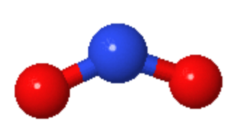


SO_2 has three regions of electrons around the central sulfur where one is a lone pair, so it has a trigonal planar electron domain geometry and a bent molecular geometry. SO_3 is a trigonal planar in electron domain geometry and molecular geometry. These molecules are dissolved in water droplets (aerosols and rain) to form sulfurous, H_2SO_3, and sulfuric, H_2SO_4, acids, resulting in acid rain which is damaging to the environment and to the human respiratory system. This environmental problem has been largely solve by removing sulfur from fuels before combustion or by removing SO_2 from flue gases using scrubbers where substances like calcium oxide (CaO) are used to convert the SO_2 gas into $CaSO_3$, an ionic solid.

Nitrogen monoxide, NO, is a gaseous molecular compound that is a pollutant formed when high temperature combustion reactions, such as those that take place in automobile engines and coal or natural gas fired power plants (as well as lightning), cause O_2 and N_2 in the atmosphere to react. With one nitrogen and one oxygen, the mono- prefix is used, but only with the oxygen. NO also goes by the name nitric oxide. The Lewis structure of NO, is :N=O: with a double bond, two lone pairs on the oxygen, a lone pair and a single electron on the N. The molecule is known as a radical because of the single electron. (It is necessary because the species has a odd number of electrons in total—there is no way to get an octet.) Radicals are typically reactive in order to get rid of the unpaired electron. NO can react with O_2 to form nitrogen dioxide, NO_2, a component of photochemical smog. In the atmosphere, however, the reaction is more complicated and NO_2 is formed from NO via reactions that do not directly involved O_2. NO can also react with O_2 and H_2O to produce nitric acid, HNO_3, which can also lead to acid rain. NO is removed from automobile exhaust with catalytic converters where it turned back into N_2 and O_2. Similar devices operate in power plants.

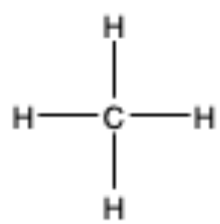
Nitrogen dioxide, NO_2, is a gaseous molecular compound that is a pollutant formed by the reaction of two NO molecules with O_2. One nitrogen (without the prefix) and two oxygen atoms gives the name, nitrogen dioxide. The Lewis structure of NO_2 (shown below) has a central nitrogen with a double bond to one oxygen and a single bond to the other. NO_2 is also a radical

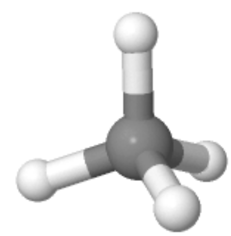




with a single electron on the nitrogen. NO_2 is what gives the brown or reddish orange color to smog. It also reacts with water to give HNO_3. HNO_3 is produced industrial from NO_2 and H_2O ($4NO_2 + 2H_2O \rightarrow 2HNO_3 + NO + NO_2 + H_2O$). NO_2 reacts with metal oxides to form nitrates (NO_3^-). The NO to NO_2 to NO_3^- series is one of the natural routes of nitrogen fixation.

Methane, CH_4, is a gaseous molecular compound and is the simplest hydrocarbon (molecules containing carbon and hydrogen). It does not follow conventional binary molecular compound naming rules but organic chemistry naming rules, where it is known as methane (meth– being the prefix for one carbon compounds and –ane being the suffix for alkanes, a class of hydrocarbons with only carbon-carbon single bonds. The Lewis structure of CH_4 has 4 hydrogen atoms connected to the central carbon atom. The molecular shape of CH_4 is tetrahedral, a three-dimensional shape that looks like a camera on a tripod. Don't be fooled by the planar appearance of the Lewis structure. The Lewis structure and molecular shape of CH_4 are shown below. CH_4 is the major component of natural gas, the fossil fuel used in home/

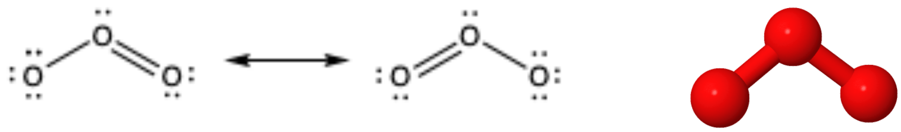




business heating and cooking and natural gas power plants. Its primary presence in the atmosphere is due to leakage from natural gas wells, pipelines, and other components of infrastructure. CH_4 is also released from the action of bacteria in the stomaches of livestock and and anaerobic decomposition of biological materials in wetlands (and landfills). CH_4 is a greenhouse gas that is the second largest contributor to atmospheric warming. Ultimately, CH_4 in the atmosphere is converted to CO_2.

Dinitrogen monoxide, N_2O, is a gaseous molecular compound is a pollutant that comes from nitrogen containing fertilizers and livestock manure. With two nitrogens at the beginning we use the prefix di- and one oxygen as the second listed element we use the prefix mono- to give the name, dinitrogen monoxide. N_2O is also called nitrous oxide, using an older naming system. It is also known as laughing gas and is used in dentistry as an anesthetic. The Lewis structure of N_2O is :N=N=O: and is a linear molecule (like CO_2). N_2O is worthy of note because it is a potent greenhouse gas. It is third after CO_2 and CH_4 as an anthropogenic (human-caused) contributor to atmospheric warming.

Ozone, O_3, is an allotrope of the element oxygen. In the stratosphere (upper atmosphere) is an important compound that protects the earth from dangerous ultraviolet (UV) radiation. In the troposphere (lower atmosphere nearest to the surface of the earth) it is a pollutant, a component of photochemical smog that causes respiratory problems in humans. The Lewis structure of O_3 is shown below, a central oxygen atom with a lone pair, a double bond to another oxygen, and a single bond to the third oxygen. O_3 is in the trigonal planar electron domain geometry and has a bent molecular shape (similar to SO_2). In the stratosphere O_3 is



formed from O_2 and O. Monatomic oxygen, O, was formed by the breaking of the O=O double bond in diatomic oxygen due to the absorption of a photon of UV light. O_3 decomposes into O_2 and O when it absorbs a photon of UV light. O_3 is formed in the troposphere by a complex series of reactions involving sunlight, NO_2, O_2, and volatile organic compounds.

Hydroxyl radical, •OH, is a very minor component of the troposphere but important in the chemistry of photochemical smog. O_3 photochemically decomposes into O_2 and an excited, reactive monatomic O. The O reacts with water to produce two •OH. •OH is involved in the reactions that lead to the conversion of NO to NO_2 and the formation of O_3.

WATER

Water is found in the earth's oceans, surface freshwater lakes and rivers, underground freshwater aquifers, water vapor in the earth's atmosphere, and as ice in the polar caps, glaciers, and snow-capped regions of the earth. It is also found in surface soils and makes up 60-70% of living organisms. Water is a compound, a pure substance with unique properties made from two or more elements found in definite proportion by mass. The formula for water is H_2O with the two hydrogens attached to the central oxygen, illustrating the general bonding principle that oxygen usually makes two bonds and hydrogen one. Water is a V-shaped molecule. By formal naming rules water would be called dihydrogen monoxide, but officially it is one of a few compounds with common names. It is simply called water.

Water dissolves many ionic compounds and polar molecules, which is one reason it is so important in biological systems. It is the matrix of moving molecules around in cells, tissues, organs, organisms, and the environment. Sea water has many dissolved ions (mostly ordinary table salt (NaCl)) and cannot be used by terrestrial biological systems which require freshwater. The limited supply of freshwater and the pollution of freshwater sources by toxic substances are two important sustainability related issues concerning water. The water cycle is a geochemical cycle on earth where liquid water evaporates into the atmosphere and then condenses in the form of rain and snow. Water is a greenhouse gas (a gas in the atmosphere that traps infrared radiation and heats the planet). Water has a high heat capacity which makes it a good coolant and moderator of the ambient temperature.

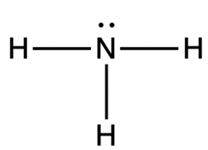
Sodium chloride, NaCl, is the second most abundant component of sea water at 3.5%. NaCl is also ordinary table salt. NaCl is an ionic compound. As a compound it is a pure substance with unique properties made from two or more elements (sodium and chlorine) found in definite proportion by mass. An ionic compound is a compound formed by the attraction of oppositely charged ions. Ions are charged particles (in this case charged atoms), which have either lost an electron to form a positive ion (Na^+ in NaCl) or gained an electron to form a negative ion (Cl^- in NaCl). NaCl(s) (the s in parenthesis tells us what state of matter (solid, liquid, gas, or aqueous) the substance is in) exists as a three-dimensional lattice with alternating positive sodium ions and negative chloride ions. When dissolved in water (NaCl(aq) or Na^+(aq) and Cl^-(aq), the ions separate from each other and are suspending in water by being surrounded by polar water molecules. Other ions are found in sea water at lower concentrations (Mg^{2+}, SO_4^{2-}, Ca^{2+}, K^+). Atmospheric gases and some organic compounds are also found in sea water.

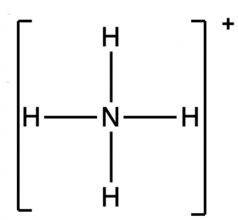
EARTH

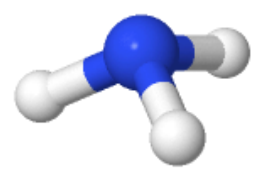
The Earth's crust is the outer, rocky layer that extends from 0-100 km deep. Oxygen is the most abundant element at 46% with silicon (27.7%), aluminum (8.2%), iron (4.1%), and calcium (3.6%) making up the top 5 elements. Most of the Earth's crust is made of minerals that are mostly silicates, polyatomic ions containing silicon and oxygen. Many of the minerals are aluminum silicates. Quartz, with an empirical formula of SiO_2 is another important silicon and oxygen containing mineral. Quartz is the main component of most sands. Quartz is used to make the pure silicon used in solar cells and computer chips. These silicon containing compounds are the main inorganic component of soil. One of the ingredient in glass is SiO_2. Iron/steel and aluminum are important materials in the modern industrial and built world. Iron is obtained from iron ores such as hematite, Fe_2O_3, and magnetite, Fe_3O_4. Aluminum is found in the rock bauxite which consists of various aluminum containing minerals. Another important material in the world today is concrete made from sand, gravel, and calcium oxide (cement), CaO, which was produced from the thermal decomposition of limestone, $CaCO_3$. This process produces the second largest amount of atmospheric CO_2 after fossil fuel combustion.

OTHER IMPORTANT SIMPLE COMPOUNDS

Ammonia/ammonium, NH_3/NH_4^+, is a gaseous, molecular compound that is primarily obtained through an industrial process called the Haber process, where N_2 is combined under high temperature and pressure with H_2 (obtained from CH_4). The Lewis structure and molecular structure of ammonia is shown below. Ammonia has three single bonds to hydrogen atoms



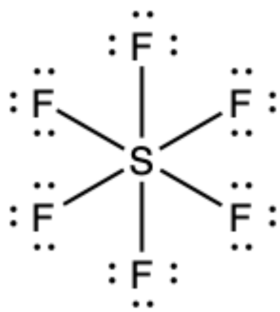


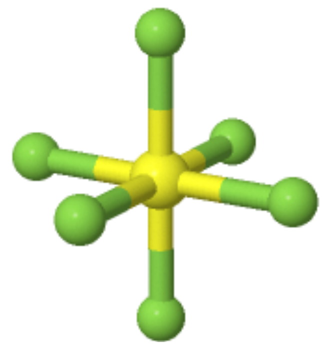


from the central nitrogen atom and one lone pair on the central nitrogen. Ammonia is highly soluble in water and is basic. In water it becomes the ammonium ion, NH_4^+, and forms the basic solution ammonium hydroxide. Ammonia and ammonium compounds are important fertilizers in agriculture.

Chlorofluorocarbons, CFCs, are a class of compounds where the hydrogens of CH_4, have been substituted with chlorine and/or fluorine atoms. Freon-12, CF_2Cl_2, is an example. These molecules were used as refrigerants and propellents, until it was discovered that they catalyzed the decomposition of O_3 from the stratosphere, after which they were banned by the international Montreal Protocol in 1987. They have been replace, largely, by hydrochlorofluorocarbons, HCFCs, where one or more of the halogen atoms is replaced by a hydrogen. Some HCFCs are based on ethane, C_2H_6, the two carbon alkane. CFCs and HCFCs are also potent greenhouse gases, and so even HCFCs are being phased out. Halons are similar molecules that contain bromine in addition to fluorine and chlorine. Halons are commonly used as fire retardants.

Sulfur hexafluoride, SF_6, is a gaseous, molecular compound is used in the electrical power industry as a gaseous insulator and arc suppressant. We include it in this list because it is also a potent anthropogenic greenhouse gas, 23,900 times that of CO_2 with an atmosphere lifetime of 800-3200 years. The Lewis structure and molecular structure of SF6 are shown below. There are 6 single bonds from the central S atom to the 6 F atoms. This structure is an exception to the octet rule, i.e we say that S has an expanded octet. Sulfur is in Period 3 of the Periodic Table where *d* orbitals are available for bonding. This allows for more than 4 bonds. Sulfur has an octahedral structure.





FIRE

Having listed air, water, and earth, three of the four elements from the ancient Greeks, it seems fitting to mention fire, the fourth one. In modern chemistry we will associate fire with the concept of energy. Energy is discussed throughout the General Chemistry course, but it comes into sharper focus in the discussion of thermochemistry, energy changes associated with chemical reactions, that occurs later in the course. We mentioned earlier the combustion of CH_4 with CO_2 as a combustion product. Typically, the main product we are interested in is the fire—the heat produced to power our world.

LEARNING GOALS

1. Identify the environmental and sustainability importance of the substances listed in this Sustainability Profile: N_2, O_2, H_2O, CO_2, CO, SO_2, SO_3, NO, NO_2, CH_4, N_2O, O_3, OH, NaCl, silicates, SiO_2, Fe_2O_3, Fe_3O_4, bauxite, $CaCO_3$, NH_3, CFC, HCFC, SF_6. (You do not need to know at this point in the course other aspects discussed such as nomenclature, Lewis structures, molecule shape. However, when these topics come up later in the course and there are specific assoicated learning goals, you should refer back to this Sustainability Profile as examples.)
2. Memorize the main components of air and their relative percentage (N_2, O_2, H_2O, Ar, CO_2). Distinguish between air and dry air.
3. List the common air pollutants (CO, SO_2, SO_3, NO, NO_2, N_2O, CH_4, N_2O, O_3, OH).
4. Explain the difference between freshwater and sea water.
5. Classify each substance discussed in this Sustainability Profile as being an element, a compound, or a mixture.

STUDY QUESTIONS

1. How can you tell the difference between an element and a compound based on the chemical formula?

2. Use substances from this Sustainability Profile to explain the difference between a mixture and a compound.
3. Which of the following are greenhouse gases: O_2, N_2, CO_2, H_2O, Ar, CH_4, $CHClF_2$?
4. What is the role of a catalytic converter in a car engine exhaust?
5. What are the three most abundant gases in dry air?
6. How is NO formed?
7. What are the different roles of the element silicon, the second most abundant element by mass on Earth?
8. Compare the structure of methane with that of CFCs and HCFCs.
9. Why would we measure atmospheric CO_2 concentrations in parts per million (ppm) rather than percent?
10. What is photochemical smog?