Hydrogen

Contents :

1 . Introdcution :

Hydrogen is the chemical element with atomic number 1 . It is represented by the symbol **H**. At standard temperature and pressure, hydrogen is a colorless, odorless, nonmetallic, tasteless, highly flammable diatomic gas with the molecular formula H_2. With an atomic weight of 1.00794 u, hydrogen is the lightest element.

- Hydrogen is the most abundant chemical element, constituting roughly 75 % of the universe's elemental mass. Stars in the main sequence are mainly composed of hydrogen in its plasma state. Elemental hydrogen is relatively rare on Earth. Industrial production is from hydrocarbons such as methane with most being used "captively" at the production site. The two largest uses are in fossil fuel processing (e.g., hydrocracking) and ammonia production mostly for the fertilizer market. Hydrogen may be produced from water by electrolysis at substantially greater cost than production from natural gas .

- The most common isotope of hydrogen is protium (name rarely used, symbol H) with a single proton and no neutrons. In ionic compounds it can take a negative charge (an anion known as a hydride and written as H^-) , or as a positively - charged species H^+. The latter cation is written as though composed of a bare proton, but in reality, hydrogen cations in ionic compounds always occur as more complex species. Hydrogen forms compounds with most elements and is present in water and most organic compounds. It plays a particularly important role in acid-base chemistry with many reactions exchanging protons between soluble molecules. As the only neutral atom with an analytic solution to the Schrödinger equation, the study of the energetics and bonding of the hydrogen atom played a key role in the development of quantum mechanics.
- Hydrogen is important in metallurgy as it can embrittle many metals, complicating the design of pipelines and storage tanks. Hydrogen is highly soluble in many rare earth and transition metals and is soluble in both nanocrystalline and amorphous metals. Hydrogen solubility in metals is influenced by local distortions or impurities in the crystal lattice.

Appearance	
colorless gas	
General	
Name, symbol, number	hydrogen, H, 1
Element category	nonmetal
Group, period, block	1, 1, s
Standard atomic weight	1.00794 (7) $g \cdot mol^{-1}$

Electron configuration	$1s^1$
Electrons per shell	1
Physical properties	
Phase	gas
Density	(0 °C , 101.325 kPa) 0.08988 g / L
Melting point	−259.14 °C
boiling point	−252.87 ° C
Triple point	- 259 °C
Critical point	32.97 K, 1.293 MPa
Heat of fusion	(H_2) 0.117 kJ·mol^{-1}
Heat of vaporization	(H_2) 0.904 kJ· mol^{-1}
Specific heat capacity	(25 °C) (H_2) 28.836 J · mol^{-1} ·K^{-1}
Atomic properties	
Oxidation states	**1** , −1(amphoteric oxide)
Electronegativity	2.20 (Pauling scale)
Ionization energies	1 st : 1312.0 kJ · mol $^{-1}$
Covalent radius	31 ± 5 pm
Van der Waals radius	120 pm
Miscellaneous	
Crystal structure	Hexagonal
Magnetic ordering	diamagnetic[1]
Thermal conductivity	(300 K) 180.5 m W·m^{-1}·K^{-1}
Speed of sound	(gas, 27 °C) 1310 m/s
CAS registry number	1333 – 74 – 0
Most stable isotopes	

Main article: Isotopes of hydrogen

iso	**N.A.**	**half-life**	**DM**	**DE (MeV)**	**DP**
^{1}H	99.985%	^{1}H is stable with 0 neutrons			

^{2}H	0.015%	^{2}H is stable with 1 neutron			
^{3}H	trace	12.32 y	β^{-}	0.01861	^{3}He

2 . Combustion

Hydrogen gas (dihydrogen) is highly flammable and will burn in air at a very wide range of concentrations between 4 % and 75 % by volume. The enthalpy of combustion for hydrogen is −286 kJ / mol

$$2\ H_2\,(g) + O_2\,(g) \rightarrow 2\ H_2O\ (l) + 572\ kJ\ (\ 286\ kJ\ /\ mol\ )$$

Hydrogen - oxygen mixtures are explosive across a wide range of proportions. Its autoignition temperature, the temperature at which it ignites spontaneously in air, is 560 °C (1,040 °F). Pure hydrogen - oxygen flames emit ultraviolet light and are nearly invisible to the naked eye as illustrated by the faint plume of the Space Shuttle main engine compared to the highly visible plume of a Space Shuttle Solid Rocket Booster). The detection of a burning hydrogen leak may require a flame detector; such leaks can be very dangerous. The explosion of the Hindenburg airship was an infamous example of hydrogen combustion; the cause is debated, but the visible flames were the result of combustible materials in the ship's skin.[14] Because hydrogen is buoyant in air, hydrogen flames tend to ascend rapidly and cause less damage than hydrocarbon fires. Two - thirds of the Hindenburg passengers survived the fire, and many deaths were instead the result of falls or burning diesel fuel.

H_2 reacts with every oxidizing element. Hydrogen can react spontaneously and violently at room temperature with chlorine and fluorine to form the corresponding halides: hydrogen chloride and hydrogen fluoride.

3 . Electron energy levels of Hydrogen atom :

Depiction of a hydrogen atom showing the diameter as about twice the Bohr model radius .

The ground state energy level of the electron in a hydrogen atom is −13.6 eV, which is equivalent to an ultraviolet photon of roughly 92 nm.

The energy levels of hydrogen can be calculated fairly accurately using the Bohr model of the atom, which conceptualizes the electron as "orbiting" the proton in analogy to the Earth's orbit of the sun. However, the electromagnetic force attracts electrons and protons to one another, while planets and celestial objects are attracted to each other by gravity. Because of the discretization of angular momentum postulated in early quantum mechanics by Bohr, the electron in the Bohr model can only occupy certain allowed distances from the proton, and therefore only certain allowed energies.

A more accurate description of the hydrogen atom comes from a purely quantum mechanical treatment that uses the Schrödinger equation or the equivalent Feynman path integral formulation to calculate the probability density of the electron around the proton.[19]

4 . Elemental molecular forms

There exist two different spin isomers of hydrogen diatomic molecules that differ by the relative spin of their nuclei.[20] In the orthohydrogen form, the spins of the two protons are parallel and form a triplet state; in the parahydrogen form the spins are antiparallel and form a singlet. At standard temperature and pressure, hydrogen gas contains about 25 % of the para form and 75 % of the ortho form, also known as the "normal form". The equilibrium ratio of orthohydrogen to parahydrogen depends on temperature, but since the ortho form is an excited state and has a higher energy than the para form, it is unstable and cannot be purified. At very low temperatures, the equilibrium state is composed almost exclusively of the para form. The liquid and gas phase thermal properties of pure parahydrogen differ significantly from those of the normal form because of differences in rotational heat capacities, as discussed more fully in Spin isomers of hydrogen. The ortho/para distinction also occurs in other hydrogen - containing molecules or functional groups, such as water and methylene, but is of little significance with respect to thermal properties.

The uncatalyzed interconversion between para and ortho H_2 increases with increasing temperature; thus rapidly condensed H_2 contains large quantities of the high - energy ortho form that convert to the para form very slowly. The ortho/para ratio in condensed H_2 is an important consideration in the preparation and storage of liquid hydrogen: the conversion from ortho to para is exothermic and produces enough heat to evaporate the hydrogen liquid, leading to loss of the liquefied material. Catalysts for the ortho - para interconversion, such as ferric oxide, activated carbon, platinized asbestos, rare earth metals, uranium compounds, chromic oxide, or some nickel compounds, are used during hydrogen cooling.

A molecular form called protonated molecular hydrogen, or H_3^+, is found in the interstellar medium (ISM), where it is generated by ionization of molecular hydrogen from cosmic rays. It has also been observed in the upper atmosphere of the planet Jupiter. This molecule is relatively stable in the environment of outer space due to the low temperature and density. H_3^+ is one of the most abundant ions in the Universe, and it plays a notable role in the chemistry of the interstellar medium.

5 . Hydrogen compounds

5 . 1 . Covalent and organic compounds

While H_2 is not very reactive under standard conditions, it does form compounds with most elements. Millions of hydrocarbons are known, but they are not formed by the direct reaction of elementary hydrogen and carbon. Hydrogen can form compounds with elements that are more electronegative, such as halogens (e.g., F, Cl, Br, I); in these compounds hydrogen takes on a partial positive charge.[28] When bonded to fluorine, oxygen, or nitrogen, hydrogen can participate in a form of strong noncovalent bonding called hydrogen bonding, which is critical to the stability of many biological molecules . Hydrogen also forms compounds with less electronegative elements, such as the metals and metalloids, in which it takes on a partial negative charge. These compounds are often known as hydrides.[31]

Hydrogen forms a vast array of compounds with carbon. Because of their general association with living things, these compounds came to be called organic compounds; the study of their properties is known as organic chemistry and their study in the context of living organisms is known as biochemistry. By some definitions, "organic" compounds are only required to contain carbon. However, most of them also contain hydrogen, and since it is the carbon-hydrogen bond which gives this class of compounds most of its particular chemical characteristics, carbon - hydrogen bonds are required in some definitions of the word "organic" in chemistry.

In inorganic chemistry, hydrides can also serve as bridging ligands that link two metal centers in a coordination complex. This function is particularly common in group 13 elements, especially in boranes (boron hydrides) and aluminium complexes, as well as in clustered carboranes.

5 . 2 . Hydrides

Compounds of hydrogen are often called hydrides, a term that is used fairly loosely. The term "hydride" implies that the H atom has acquired a negative or anionic character, denoted H^-, and is used when hydrogen forms a compound with a more electropositive element. The existence of the hydride anion, suggested by Gilbert N. Lewis in 1916 for group I and II salt-like hydrides, was demonstrated by Moers in 1920 with the electrolysis of molten lithium hydride (LiH), that produced a stoichiometric quantity of hydrogen at the anode.[36] For hydrides other than group I and II metals, the term is quite misleading, considering the low electronegativity of hydrogen. An exception in group II hydrides is BeH_2, which is polymeric. In lithium aluminium hydride, the AlH_4^- anion carries hydridic centers firmly attached to the Al (III) . Although hydrides can be formed with almost all main-group elements, the number and combination of possible compounds varies widely; for example, there are over 100 binary borane hydrides known, but only one binary aluminium hydride. Binary indium hydride has not yet been identified, although larger complexes exist.

5 . 3 . Protons and acids

Oxidation of hydrogen, in the sense of removing its electron, formally gives H^+, containing no electrons and a nucleus which is usually composed of one proton. That is why H^+ is often called a proton. This species is central to discussion of acids. Under the Bronsted-Lowry theory, acids are proton donors, while bases are proton acceptors.

A bare proton H^+ cannot exist in solution or in ionic crystals, because of its unstoppable attraction to other atoms or molecules with electrons. Except at the high temperatures associated with plasmas, such protons cannot be removed from the electron clouds of atoms and molecules, and will remain attached to them. However, the term 'proton' is sometimes used loosely and metaphorically to refer to positively charged or cationic hydrogen attached to other species in this fashion, and as such is denoted "H^+" without any implication that any single protons exist freely as a species.

To avoid the implication of the naked "solvated proton" in solution, acidic aqueous solutions are sometimes considered to contain a less unlikely fictitious species, termed the "hydronium ion" (H_3O^+). However, even in this case, such solvated hydrogen cations are thought more realistically physically to be organized into clusters that form species closer to $H_9O_4^+$. Other oxonium ions are found when water is in solution with other solvents.

Although exotic on earth, one of the most common ions in the universe is the H_3^+ ion, known as protonated molecular hydrogen or the triatomic hydrogen cation.

6 . Isotopes of hydrogen

Protium, the most common isotope of hydrogen, has one proton and one electron. Unique among all stable isotopes, it has no neutrons .

Hydrogen has three naturally occurring isotopes, denoted ^{1}H, ^{2}H, and ^{3}H. Other, highly unstable nuclei (^{4}H to ^{7}H) have been synthesized in the laboratory but not observed in nature.

- **^{1}H** is the most common hydrogen isotope with an abundance of more than 99.98 %. Because the nucleus of this isotope consists of only a single proton, it is given the descriptive but rarely used formal name *protium*.
- **^{2}H**, the other stable hydrogen isotope, is known as *deuterium* and contains one proton and one neutron in its nucleus. Essentially all deuterium in the universe is thought to have been produced at the time of the Big Bang, and has endured since that time. Deuterium is not radioactive, and does not represent a significant toxicity hazard. Water enriched in molecules that include deuterium instead of normal hydrogen is called heavy water. Deuterium and its compounds are used as a non -radioactive label in chemical experiments and in solvents for ^{1}H-NMR spectroscopy. Heavy water is used as a neutron moderator and coolant for nuclear reactors. Deuterium is also a potential fuel for commercial nuclear fusion.
- **^{3}H** is known as *tritium* and contains one proton and two neutrons in its nucleus. It is radioactive, decaying into Helium -3 through beta decay with a half - life of 12.32 years. Small amounts of tritium occur naturally because of the interaction of cosmic rays with atmospheric gases; tritium has also been released during nuclear weapons tests. It is used in nuclear fusion reactions,[48] as a tracer in isotope geochemistry, and specialized in self-powered lighting devices. Tritium has also been used in chemical and biological labeling experiments as a radiolabel.

Hydrogen is the only element that has different names for its isotopes in common use today. (During the early study of radioactivity, various heavy radioactive isotopes were given names, but such names are no longer used). The symbols D and T (instead of ^{2}H and ^{3}H) are sometimes used for deuterium and tritium, but the corresponding symbol P is already in use for phosphorus and thus is not available for protium. In its nomenclatural guidelines, the

International Union of Pure and Applied Chemistry allows any of D, T, ^2H, and ^3H to be used, although ^2H and ^3H are preferred.

7 . Natural occurrence

Hydrogen is the most abundant element in the universe, making up 75 % of normal matter by mass and over 90 % by number of atoms.[54] This element is found in great abundance in stars and gas giant planets. Molecular clouds of H_2 are associated with star formation. Hydrogen plays a vital role in powering stars through proton-proton reaction and CNO cycle nuclear fusion.

Throughout the universe, hydrogen is mostly found in the atomic and plasma states whose properties are quite different from molecular hydrogen. As a plasma, hydrogen's electron and proton are not bound together, resulting in very high electrical conductivity and high emissivity (producing the light from the sun and other stars). The charged particles are highly influenced by magnetic and electric fields. For example, in the solar wind they interact with the Earth's magnetosphere giving rise to Birkeland currents and the aurora. Hydrogen is found in the neutral atomic state in the Interstellar medium. The large amount of neutral hydrogen found in the damped Lyman-alpha systems is thought to dominate the cosmological baryonic density of the Universe up to redshift $z = 4$.

Under ordinary conditions on Earth, elemental hydrogen exists as the diatomic gas, H_2 (for data see table). However, hydrogen gas is very rare in the Earth's atmosphere (1 ppm by volume) because of its light weight, which enables it to escape from Earth's gravity more easily than heavier gases. However, hydrogen (in chemically combined form) is the third most abundant element on the Earth's surface.[57] Most of the Earth's hydrogen is in the form of chemical compounds such as hydrocarbons and water.[35] Hydrogen gas is produced by some bacteria and algae and is a natural component of flatus. Methane is a hydrogen source of increasing importance.

8 . History

8 . 1 .Discovery and use

Hydrogen gas, H_2, was first artificially produced and formally described by T. Von Hohenheim (also known as Paracelsus, 1493 – 1541) via the mixing of metals with strong acids.[59] He was unaware that the flammable gas produced by this chemical reaction was a new chemical element. In 1671, Robert Boyle rediscovered and described the reaction between iron filings and dilute acids, which results in the production of hydrogen gas. In 1766, Henry Cavendish was the first to recognize hydrogen gas as a discrete substance, by identifying the gas from a metal-acid reaction as "inflammable air" and further finding in 1781 that the gas produces water when burned. He is usually given credit for its discovery as an element. In 1783, Antoine Lavoisier gave the element the name hydrogen (from the Greek *hydro* meaning water and *genes* meaning creator) when he and Laplace reproduced Cavendish's finding that water is produced when hydrogen is burned.

Hydrogen was liquefied for the first time by James Dewar in 1898 by using regenerative cooling and his invention, the vacuum flask.[62] He produced solid hydrogen the next year. Deuterium was discovered in December 1931 by Harold Urey, and tritium was prepared in 1934 by Ernest Rutherford, Mark Oliphant, and Paul Harteck.[61] Heavy water, which consists of deuterium in the place of regular hydrogen, was discovered by Urey's group in 1932. François Isaac de Rivaz built the first internal combustion engine powered by a mixture of hydrogen and oxygen in 1806. Edward Daniel Clarke invented the hydrogen gas blowpipe in 1819. The Döbereiner's lamp and limelight were invented in 1823.

The first hydrogen-filled balloon was invented by Jacques Charles in 1783. Hydrogen provided the lift for the first reliable form of air-travel following the 1852 invention of the first hydrogen-lifted airship by Henri Giffard. German count Ferdinand von Zeppelin promoted the idea of rigid airships lifted by hydrogen that later were called Zeppelins; the first of which had its maiden flight in 1900.[62]

Regularly scheduled flights started in 1910 and by the outbreak of World War I in August 1914, they had carried 35,000 passengers without a serious incident. Hydrogen - lifted airships were used as observation platforms and bombers during the war.

The first non - stop transatlantic crossing was made by the British airship *R34* in 1919. Regular passenger service resumed in the 1920s and the discovery of helium reserves in the United States promised increased safety, but the U.S. government refused to sell the gas for this purpose. Therefore, H_2 was used in the *Hindenburg* airship, which was destroyed in a midair fire over New Jersey on May 6, 1937.

The incident was broadcast live on radio and filmed. Ignition of leaking hydrogen as widely assumed to be the cause but later investigations pointed to ignition of the aluminized fabric coating by static electricity. But the damage to hydrogen's reputation as a lifting gas was already done. In the same year the first hydrogen-cooled turbogenerator went into service with gaseous hydrogen as a coolant in the rotor and the stator in 1937 at Dayton, Ohio, by the Dayton Power & Light Co,[64] because of the thermal conductivity of hydrogen gas this is the most common type in its field today. The nickel hydrogen battery was used for the first time in 1977 aboard the U.S. Navy's Navigation technology satellite-2 (NTS - 2). For example, the ISS, Mars Odyssey and the Mars Global Surveyor are equipped with nickel - hydrogen batteries. The Hubble Space Telescope, at the time its original batteries were finally changed in May 2009, more than 19 years after launch, led with the highest number of charge/discharge cycles of any NiH2 battery in low earth orbit.

8 . 1 . Role in quantum theory

Hydrogen emission spectrum lines in the visible range. These are the four visible lines of the Balmer series

Because of its relatively simple atomic structure, consisting only of a proton and an electron, the hydrogen atom, together with the spectrum of light produced from it or absorbed by it, has been central to the development of the theory of atomic structure.[70] Furthermore, the corresponding simplicity of the hydrogen molecule and the corresponding cation H_2^+ allowed fuller understanding of the nature of the chemical bond, which followed shortly after the quantum mechanical treatment of the hydrogen atom had been developed in the mid – 1920 s .

One of the first quantum effects to be explicitly noticed (but not understood at the time) was a Maxwell observation involving hydrogen, half a century before full quantum mechanical theory arrived. Maxwell observed that the specific heat capacity of H_2 unaccountably departs from that of a diatomic gas below room temperature and begins to increasingly resemble that of a monatomic gas at cryogenic temperatures. According to quantum theory, this behavior arises from the spacing of the (quantized) rotational energy levels, which are particularly wide - spaced in H_2 because of its low mass. These widely spaced levels inhibit equal partition of heat energy into rotational motion in hydrogen at low temperatures. Diatomic gases composed of heavier atoms do not have such widely spaced levels and do not exhibit the same effect.

9 . Production

H_2 is produced in chemistry and biology laboratories, often as a by-product of other reactions; in industry for the hydrogenation of unsaturated substrates; and in nature as a means of expelling reducing equivalents in biochemical reactions.

9 . 1 . Laboratory

In the laboratory, H_2 is usually prepared by the reaction of acids on metals such as zinc with Kipp's apparatus.

$$Zn + 2\ H^+ \rightarrow Zn^{2+} + H_2$$

Aluminium can also produce H_2 upon treatment with bases:

$$2\ Al + 6\ H_2O + 2\ OH^- \rightarrow 2\ Al(OH)_4^- + 3\ H_2$$

The electrolysis of water is a simple method of producing hydrogen. A low voltage current is run through the water, and gaseous oxygen forms at the anode while gaseous hydrogen forms at the cathode. Typically the cathode is made from platinum or another inert metal when producing hydrogen for storage. If, however, the gas is to be burnt on site, oxygen is desirable to assist the combustion, and so both electrodes would be made from inert metals. (Iron, for instance, would oxidize, and thus decrease the amount of oxygen given off.) The theoretical maximum efficiency (electricity used vs. energetic value of hydrogen produced) is between 80 – 94 %.

$$2H_2O\ (aq) \rightarrow 2H_2\ (g) + O_2\ (g)$$

In 2007, it was discovered that an alloy of aluminium and gallium in pellet form added to water could be used to generate hydrogen. The process also creates alumina, but the expensive gallium, which prevents the formation of an oxide skin on the pellets, can be re-used. This has important potential implications for a hydrogen economy, since hydrogen can be produced on-site and does not need to be transported.

9 . 2 . Industrial

Hydrogen can be prepared in several different ways, but economically the most important processes involve removal of hydrogen from hydrocarbons. Commercial bulk hydrogen is usually produced by the steam reforming of natural gas. At high temperatures (700 –1100 °C) , steam (water vapor) reacts with methane to yield carbon monoxide and H_2.

$$CH_4 + H_2O \rightarrow CO + 3\ H_2$$

This reaction is favored at low pressures but is nonetheless conducted at high pressures (20 atm; 600 inHg) since high pressure H_2 is the most marketable product. The product mixture is known as "synthesis gas" because it is often used directly for the production of methanol and related compounds. Hydrocarbons other than methane can be used to produce synthesis gas with varying product ratios. One of the many complications to this highly optimized technology is the formation of coke or carbon:

$$CH_4 \rightarrow C + 2\,H_2$$

Consequently, steam reforming typically employs an excess of H_2O. Additional hydrogen can be recovered from the steam by use of carbon monoxide through the water gas shift reaction, especially with an iron oxide catalyst. This reaction is also a common industrial source of carbon dioxide:[74]

$$CO + H_2O \rightarrow CO_2 + H_2$$

Other important methods for H_2 production include partial oxidation of hydrocarbons:

$$2\,CH_4 + O_2 \rightarrow 2\,CO + 4\,H_2$$

and the coal reaction, which can serve as a prelude to the shift reaction above:

$$C + H_2O \rightarrow CO + H_2$$

Hydrogen is sometimes produced and consumed in the same industrial process, without being separated. In the Haber process for the production of ammonia, hydrogen is generated from natural gas.[76] Electrolysis of brine to yield chlorine also produces hydrogen as a co-product.

9 . 3 . Thermo Chemical

There are more than 200 thermochemical cycles which can be used for water splitting, around a dozen of these cycles such as the iron oxide cycle, cerium (IV) oxide-cerium (III) oxide cycle, zinc zinc-oxide cycle, sulfur-iodine cycle, copper-chlorine cycle and hybrid sulfur cycle are under research and in testing phase to produce hydrogen and oxygen from water and heat without using electricity . A number of laboratories (including in France, Germany, Greece, Japan, and the USA) are developing thermochemical methods to produce hydrogen from solar energy and water.

10 . Applications

Large quantities of H_2 are needed in the petroleum and chemical industries. The largest application of H_2 is for the processing ("upgrading") of fossil fuels, and in the production of ammonia. The key consumers of H_2 in the petrochemical plant include hydrodealkylation, hydrodesulfurization, and hydrocracking. H_2 has several other important uses. H_2 is used as a hydrogenating agent, particularly in increasing the level of saturation of unsaturated fats and oils (found in items such as margarine), and in the production of methanol. It is similarly the source of hydrogen in the manufacture of hydrochloric acid. H_2 is also used as a reducing agent of metallic ores.

Apart from its use as a reactant, H_2 has wide applications in physics and engineering. It is used as a shielding gas in welding methods such as atomic hydrogen welding . H_2 is used as the rotor coolant in electrical generators at power stations, because it has the highest thermal conductivity of any gas. Liquid H_2 is used in cryogenic research, including superconductivity studies. Since H_2 is lighter than air, having a little more than 1/15th of the density of air, it was once widely used as a lifting gas in balloons and airships.[84]

In more recent applications, hydrogen is used pure or mixed with nitrogen (sometimes called forming gas) as a tracer gas for minute leak detection. Applications can be found in the automotive, chemical, power generation, aerospace, and telecommunications industries . Hydrogen is an authorized food additive (E 949) that allows food package leak testing among other anti - oxidizing properties.

Hydrogen's rarer isotopes also each have specific applications. Deuterium (hydrogen-2) is used in nuclear fission applications as a moderator to slow neutrons, and in nuclear fusion reactions.[62] Deuterium compounds have applications in chemistry and biology in studies of reaction isotope effects. Tritium (hydrogen-3), produced in nuclear reactors, is used in the production of hydrogen bombs,[88] as an isotopic label in the biosciences, and as a radiation source in luminous paints.

The triple point temperature of equilibrium hydrogen is a defining fixed point on the ITS - 90 temperature scale at 13.8033 kelvins .

10 . 1 . Energy carrier

Hydrogen is not an energy resource, except in the hypothetical context of commercial nuclear fusion power plants using deuterium or tritium, a technology presently far from development. The Sun's energy comes from nuclear fusion of hydrogen, but this process is difficult to achieve controllably on Earth.[Elemental hydrogen from solar, biological, or electrical sources require more energy to make it than is obtained by burning it, so in these cases hydrogen functions as an energy carrier, like a battery. Hydrogen may be obtained from fossil sources (such as methane), but these sources are unsustainable.

The energy density per unit *volume* of both liquid hydrogen and compressed hydrogen gas at any practicable pressure is significantly less than that of traditional fuel sources, although the energy density per unit fuel *mass* is higher.[91] Nevertheless, elemental hydrogen has been widely discussed in the context of energy, as a possible future *carrier* of energy on an economy-wide scale. For example, CO_2 sequestration followed by carbon capture and storage could be conducted at the point of H_2 production from fossil fuels.[95] Hydrogen used in transportation would burn relatively cleanly, with some NOx emissions, but without carbon emissions. However, the infrastructure costs associated with full conversion to a hydrogen economy would be substantial.

11 . Biological reactions

H_2 is a product of some types of anaerobic metabolism and is produced by several microorganisms, usually via reactions catalyzed by iron - or nickel - containing enzymes called hydrogenases. These enzymes catalyze the reversible redox reaction between H_2 and its component two protons and two electrons. Creation of hydrogen gas occurs in the transfer of reducing equivalents produced during pyruvate fermentation to water.

Water splitting, in which water is decomposed into its component protons, electrons, and oxygen, occurs in the light reactions in all photosynthetic organisms. Some such organisms—including the alga *Chlamydomonas reinhardtii* and cyanobacteria—have evolved a second step in the dark reactions in which protons and electrons are reduced to form H_2 gas by specialized hydrogenases in the chloroplast. Efforts have been undertaken to genetically modify cyanobacterial hydroge Efforts have also been undertaken with genetically modified alga in a bioreactor.

12 . Safety and precautions

Inhalation of air with high concentration of hydrogen as with hydrox and hydreliox displaces oxygen and may cause the above symptoms as an asphyxant.

Hydrogen poses a number of hazards to human safety, from potential detonations and fires when mixed with air to being an asphyxant in its pure, oxygen-free form. In addition, liquid hydrogen is a cryogen and presents dangers (such as frostbite) associated with very cold liquids. Hydrogen dissolves in some metals, and, in addition to leaking out, may have adverse effects on them, such as hydrogen embrittlement. Hydrogen gas leaking into external air may spontaneously ignite. Moreover, hydrogen fire, while being extremely hot, is almost invisible, and thus can lead to accidental burns.

Even interpreting the hydrogen data (including safety data) is confounded by a number of phenomena. Many physical and chemical properties of hydrogen depend on the parahydrogen/orthohydrogen ratio (it often takes days or weeks at a given temperature to reach the equilibrium ratio, for which the data is usually given). Hydrogen detonation parameters, such as critical detonation pressure and temperature, strongly depend on the container geometry.

Hydrogen peroxide

Contents

1 . Introduction :

Hydrogen peroxide (H_2O_2) is a very pale blue liquid, slightly more viscous than water, which appears colorless in dilute solution. It is a weak acid, has strong oxidizing properties, and is a powerful bleaching agent. It is used as a disinfectant, antiseptic, oxidizer, and in rocketry as a propellant. The oxidizing capacity of hydrogen peroxide is so strong that it is considered a highly reactive oxygen species.

In organisms, hydrogen peroxide is naturally produced as a byproduct of oxygen metabolism; virtually all possess enzymes known as peroxidases, which harmlessly and catalytically decompose low concentrations of hydrogen peroxide to water and oxygen.

Other Names	Dioxidane
UN Number	2015 (> 60 % soln.) 2014 (20 – 60 % soln.) 2984 (8 – 20 % soln.)
Molecular Formula	H_2O_2
Molar Mass	34.0147 g / mol
Appearance	Colorless in solution
Density	1.463 g / cm^3
Melting point	- 0.43 °C
Boiling point	150.2 °C
Solubility in Water	Miscible
Solubility	Soluble in ether
Acidity (pK_a)	11.62
Refractive index (n_D)	1.34
Viscosity	1.245 cP (20 ° C)
EU classification	Oxidant (O) Corrosive (C) Harmful (Xn)
Flash point	Non – flammable
LD_{50}	1518 mg / kg

2 . Structure and properties

As with all molecules, the physical properties of hydrogen peroxide are the result of its molecular mass, structure and distribution of atoms within the molecule.

The preferred molecular structure of any molecule is the configuration which has the lowest internal stress. For hydrogen peroxide, there are two basic structural forms (conformers) available for the molecule. While flat shape of the *anti* conformer would minimize steric repulsions, the 90 ° torsion angle of the *syn* conformer would optimize mixing between the filled *p - type* orbital of the oxygen (one of the lone pairs) and the LUMO of the vicinal O - H bond .

The resulting anticlinal " skewed " shape is a compromise between the two conformers.

Despite the fact that the O - O bond is a single bond, the molecule has a remarkably high barrier to complete rotation of 29.45 kJ / mol (compared with 12.5 kJ / mol for the rotational barrier of ethane). The increased barrier is attributed to repulsion between one lone pair and other lone pairs. The bond angles are affected by hydrogen bonding, which is relevant to the structural difference between gaseous and crystalline forms; indeed a wide range of values is seen in crystals containing molecular H_2O_2.

Comparison with analogues

Analogues of hydrogen peroxide include the chemically identical deuterium peroxide and malodorous hydrogen disulfide.[4] Hydrogen disulfide has a boiling point of only 70.7°C despite having a higher molecular weight, indicating that hydrogen bonding increases the boiling point of hydrogen peroxide.[5]

Physical properties of hydrogen peroxide solutions

Aqueous hydrogen peroxide solutions have specific properties that are different from those of the pure chemical due to hydrogen bonding between water and hydrogen peroxide molecules. Specifically, hydrogen peroxide and water form a eutectic mixture, exhibiting freezing-point depression. While pure water melts and freezes at approximately 273K , and pure hydrogen peroxide just 0.4K below that, a 50 % (by volume) solution melts and freezes at 221 K.[6]

3 . History

Hydrogen peroxide was first isolated in 1818 by Louis Jacques Thénard by reacting barium peroxide with nitric acid.[7] An improved version of this process used hydrochloric acid, followed by sulfuric acid to precipitate the barium sulfate byproduct. Thénard's process was used from the end of the 19 th century until the middle of the 20th century. Modern production methods are discussed below.

For a long time it was believed that pure hydrogen peroxide was unstable, because attempts to separate the hydrogen peroxide from the water, which is present during synthesis, failed. This was because traces of solids and heavy metal ions led to a catalytic decomposition or explosions of the hydrogen peroxide. 100 % pure hydrogen peroxide was first obtained through vacuum distillation by Richard Wolffenstein in 1894. At the end of 19 th century, Petre Melikishvili and his pupil L. Pizarjevski showed that of the many proposed formulas of hydrogen peroxide, the correct one was H-O-O-H.

The use of H_2O_2 sterilization in biological safety cabinets and barrier isolators is a popular alternative to ethylene oxide (EtO) as a safer, more efficient decontamination method. H_2O_2 has long been widely used in the pharmaceutical industry. In aerospace research, H_2O_2 is used to sterilize satellites.

The FDA has recently granted 510 (k) clearance to use H_2O_2 in individual medical device manufacturing applications. EtO criteria outlined in ANSI / AAMI / ISO 14937 may be used as a validation guideline. Sanyo was the first manufacturer to use the H_2O_2 process in situ in a cell culture incubator, which is a faster and more efficient cell culture sterilization process.

4 . Manufacture

Formerly inorganic processes were used, employing the electrolysis of an aqueous solution of sulfuric acid or acidic ammonium bisulfate (NH_4HSO_4) , followed by hydrolysis of the peroxodisulfate $((SO_4)_2)^{2-}$ which is formed.

However, today hydrogen peroxide is manufactured almost exclusively by the autoxidation of a 2 - alkyl anthrahydroquinone (or 2 - alkyl - 9 , 10 - dihydroxyanthracene) to the corresponding 2 -alkyl anthraquinone. Major producers commonly use either the 2- ethyl or the 2 - amyl derivative. The cyclic reaction depicted below, shows the

2 - ethyl derivative, where 2 – ethyl - 9 ,10 - dihydroxyanthracene ($C_{16}H_{14}O_2$), is oxidized to the corresponding 2- ethylanthraquinone ($C_{16}H_{12}O_2$) and hydrogen peroxide. Most commercial processes achieve this by bubbling compressed air through a solution of the anthracene, whereby the oxygen present in the air reacts with the labile hydrogen atoms (of the hydroxy group) giving hydrogen peroxide and regenerating the anthraquinone. Hydrogen peroxide is then extracted out and the anthraquinone derivative reduced back to the dihydroxy (anthracene) compound using hydrogen gas in the presence of a metal catalyst. The cycle then repeats itself.[10][11]

This process is known as the Riedl - Pfleiderer process[11], having been first discovered by them in 1936. The overall equation for the process is deceptively simple :

$$H_2 + O_2 \rightarrow H_2O_2$$

It is important to point out that the economics of the process depend heavily on effective recycling of the quinone (which is very expensive) and extraction solvents, and of the hydrogenation catalyst.

In 1994, world production of H_2O_2 was around 1.9 million tonnes and grew to 2.2 million in 2006 , most of which was at a concentration of 70 % or less .

4 . 1 . New developments

A new, so called " high productivity / high yield " process, based on an optimized distribution of isomers of 2 - amyl anthraquinone has been developed by Solvay. In July 2008, this process allowed the construction of a " mega " scale single - train plant in Zandvliet (Belgium). The plant has an annual production capacity more than two times that of the world's next largest single train plant. An even larger plant is scheduled to come onstream at Map Ta Phut (Thailand) in 2011. It can be imagined that this leads to reduction in the cost of production due to economies of scale.

A process to produce hydrogen peroxide directly from the elements has been of interest to producers for many years. The problem with the direct synthesis process is that thermodynamically, the reaction of hydrogen with oxygen favors production of water. It had been recognized for some time that a finely dispersed catalyst was beneficial in promoting selectivity to hydrogen peroxide but while selectivity was improved it was still not sufficiently high to permit commercial development of the process. However, an apparent breakthrough was made in the mid to late 2000s by researchers at Headwaters Technology (a self - described energy, environmental control and nanotechnology innovation company). The breakthrough revolves around development of a minute (nanometer sized) phase-controlled noble metal crystal particles on carbon support. This apparently led, in a joint venture with Evonik Industries, to the construction of a pilot plant in Germany in late 2005. The pilot plant trials to test the commercial feasibility of the process are presumably ongoing since little has been revealed about the results or progress of the operation. It is claimed that there are reductions in investment cost because the process is simpler and involves less equipment; however, the process is also more corrosive and unproven. It should be noted that this process results in low concentrations of hydrogen peroxide (about 5 - 10 wt % versus about 40 wt % through the anthraquione process), and is therefore only suitable for " over the fence " applications .

In 2009, another catalyst development was announced by workers at Cardiff University. This development also relates to the direct synthesis, but in this case, specifically using gold – palladium nanoparticles. Normally the direct synthesis must be carried out in an acid medium to prevent immediate decomposition of the hydrogen peroxide once it is formed. While hydrogen peroxide has a tendency to decompose on its own (which is why, even after production, it is often necessary to add stabilisers to the commercial product when it is to be transported or stored for long periods), the nature of the catalyst can cause this decomposition to accelerate rapidly. It is claimed that the use of this gold - palladium catalyst reduces this decomposition and consequently little to no acid is required. The process is in a very early stage of development and currently results in very low concentrations of hydrogen peroxide being formed (less than about 1–2 wt %). Nonetheless, it is envisaged by the inventors that the process will lead to an inexpensive, efficient, and environmentally friendly process .

A novel electrochemical process for the production of alkaline hydrogen peroxide has been developed by Dow. The process employs a monopolar cell to achieve an electrolytic reduction of oxygen in a dilute sodium hydroxide solution .

5 . Reactions

5 . 1 . Decomposition

Hydrogen peroxide always decomposes (disproportionates) exothermically into water and oxygen gas spontaneously:

$$2\ H_2O_2 \rightarrow 2\ H_2O + O_2$$

This process is very favorable thermodynamically. It has a $\Delta H^\ominus$ of $-98.2\ \text{kJ} \cdot \text{mol}^{-1}$ and a $\Delta G^\ominus$ of $-119.2\ \text{kJ} \cdot \text{mol}^{-1}$ and a ΔS of $70.5\ \text{J} \cdot \text{mol}^{-1} \cdot \text{K}^{-1}$. The rate of decomposition is dependent on the temperature and concentration of the peroxide, as well as the pH and the presence of impurities and stabilizers. Hydrogen peroxide is incompatible with many substances that catalyse its decomposition, including most of the transition metals and their compounds. Common catalysts include manganese dioxide, and silver. The same reaction is catalysed by the enzyme catalase, found in the liver, whose main function in the body is the removal of toxic byproducts of metabolism and the reduction of oxidative stress. The decomposition occurs more rapidly in alkali, so acid is often added as a stabilizer.

The liberation of oxygen and energy in the decomposition has dangerous side effects. Spilling high concentrations of hydrogen peroxide on a flammable substance can cause an immediate fire, which is further fueled by the oxygen released by the decomposing hydrogen peroxide. High - strength peroxide (also called high - test peroxide, or HTP) must be stored in a suitable, vented container to prevent the buildup of oxygen gas, which would otherwise lead to the eventual rupture of the container.

In the presence of certain catalysts, such as Fe^{2+} or Ti^{3+}, the decomposition may take a different path, with free radicals such as HO· (hydroxyl) and HOO· being formed. A combination of H_2O_2 and Fe^{2+} is known as *Fenton's reagent.*

A common concentration for hydrogen peroxide is " 20 volume ", which means that when 1 volume of hydrogen peroxide is decomposed, it produces 20 volumes of oxygen. A 20 "volume" concentration of hydrogen peroxide is equivalent to 1.667 mol/dm^3 (Molar solution) or about 6 %.

Hydrogen peroxide available at drug stores is three percent solution. In such small concentrations, it is less stable, and decomposes faster. It is usually stabilized with acetanilide, a substance which has toxic side effects in significant amounts.

5 . 2 . Redox reactions

H_2O_2 is one of the most powerful oxidizers known - stronger than chlorine, chlorine dioxide, and potassium permanganate. Also, through catalysis, H_2O_2 can be converted into hydroxyl radicals (.OH) with reactivity second only to fluorine.

Oxidant	**Oxidation potential , V**
Fluorine	3.0
Hydroxyl radical	2.8
Ozone	2.1
Hydrogen peroxide	1.8
Potassium permanganate	1.7
Chlorine dioxide	1.5
Chlorine	1.4

In aqueous solution, hydrogen peroxide can oxidize or reduce a variety of inorganic ions. When it acts as a reducing agent, oxygen gas is also produced. In acidic solutions Fe^{2+} is oxidized to Fe^{3+},

$$2\ Fe^{2+}(aq) + H_2O_2 + 2\ H^{+}(aq) \rightarrow 2\ Fe^{3+}(aq) + 2H_2O\ (l)$$

and sulfite (SO_3^{2-}) is oxidized to sulfate (SO_4^{2-}). However, potassium permanganate is reduced to Mn^{2+} by acidic H_2O_2. Under alkaline conditions, however, some of these reactions reverse; for example, Mn^{2+} is oxidized to Mn^{4+} (as MnO_2).

Another example of hydrogen peroxide acting as a reducing agent is the reaction with sodium hypochlorite, which is a convenient method for preparing oxygen in the laboratory.

$$NaOCl + H_2O_2 \rightarrow O_2 + NaCl + H_2O$$

Hydrogen peroxide is frequently used as an oxidizing agent in organic chemistry. One application is for the oxidation of thioethers to sulfoxides. For example, methyl phenyl sulfide was oxidized to methyl phenyl sulfoxide in 99 % yield in methanol in 18 hours (or 20 minutes using a $TiCl_3$ catalyst) :

$$Ph\text{- }S\text{ - }CH_3 + H_2O_2 \rightarrow Ph – S\ (O)\text{ - }CH_3 + H_2O$$

Alkaline hydrogen peroxide is used for epoxidation of electron-deficient alkenes such as acrylic acids, and also for oxidation of alkylboranes to alcohols, the second step of hydroboration-oxidation.

5 . 3 . Formation of peroxide compounds

Hydrogen peroxide is a weak acid, and it can form hydroperoxide or peroxide salts or derivatives of many metals.

For example, on addition to an aqueous solution of chromic acid (CrO_3) or acidic solutions of dichromate salts, it will form an unstable blue peroxide $Cr\,O\,(O_2)_2$. In aqueous solution it rapidly decomposes to form oxygen gas and chromium salts.

It can also produce peroxoanions by reaction with anions; for example, reaction with borax leads to sodium perborate, a bleach used in laundry detergents:

$$Na_2B_4O_7 + 4\ H_2O_2 + 2\ NaOH \rightarrow 2\ Na_2B_2O_4(OH)_4 + H_2O$$

H_2O_2 converts carboxylic acids (RCOOH) into peroxy acids (RCOOOH), which are them selves used as oxidizing agents.

Hydrogen peroxide reacts with acetone to form acetone peroxide, and it interacts with ozone to form hydrogen trioxide, also known as trioxidane. Reaction with urea produces carbamide peroxide, used for whitening teeth. An acid-base adduct with triphenylphosphine oxide is a useful " carrier " for H_2O_2 in some reactions.

5 . 4 . Alkalinity

Hydrogen peroxide is a much weaker base than water, but it can still form adducts with very strong acids. The superacid HF/SbF_5 forms unstable compounds containing the $[H_3O_2]^+$ ion.

6 . Uses

3 . 1 . Industrial applications

About 50 % of the world's production of hydrogen peroxide in 1994 was used for pulp- and paper-bleaching. Other bleaching applications are becoming more important as hydrogen peroxide is seen as an environmentally benign alternative to chlorine-based bleaches. It is highly corrosive to metal.

Other major industrial applications for hydrogen peroxide include the manufacture of sodium percarbonate and sodium perborate, used as mild bleaches in laundry detergents. It is used in the production of certain organic peroxides such as dibenzoyl peroxide, used in polymerisations and other chemical processes. Hydrogen peroxide is also used in the production of epoxides such as propylene oxide. Reaction with carboxylic acids produces a corresponding peroxy acid. Peracetic acid and meta – chloro peroxy benzoic acid (commonly abbreviated mCPBA) are prepared from acetic acid and *meta* - chloro benzoic acid, respectively. The latter is commonly reacted with alkenes to give the corresponding epoxide.

In the PCB manufacturing process, hydrogen peroxide mixed with sulfuric acid was used as the microetch chemical for copper surface roughening preparation.

A combination of a powdered precious metal-based catalyst, hydrogen peroxide, methanol and water can produce superheated steam in one to two seconds, releasing only CO_2 and high temperature steam for a variety of purposes.

Recently, there has been increased use of vaporized hydrogen peroxide in the validation and bio- decontamination of half suit and glove port isolators in pharmaceutical production.

Nuclear pressurized water reactors (PWRs) use hydrogen peroxide during the plant shutdown to force the oxidation and dissolution of activated corrosion products deposited on the fuel. The corrosion products are then removed with the cleanup systems before the reactor is disassembled.

Hydrogen peroxide is also used in the oil and gas exploration industry to oxidize rock matrix in preparation for micro - fossil analysis.

6 . 2 . Chemical applications

A method of producing propylene oxide from hydrogen peroxide has been developed. The process is claimed to be environmentally friendly since the only significant byproduct is water. It is also claimed the process has significantly lower investment and operating costs. Two of these " HPPO " (hydrogen peroxide to propylene oxide) plants came onstream in 2008: One of them located in Belgium is a Solvay, Dow - BASF joint venture, and the other in Korea, is a Evonik Head Waters, SK Chemicals joint venture. A caprolactam application for hydrogen peroxide has been commercialized. Potential routes to phenol and epichlorohydrin utilizing hydrogen peroxide have been postulated .

6 . 3 . Biological function

A study published in *Nature* found that hydrogen peroxide plays a role in the immune system. Scientists found that hydrogen peroxide is released after tissues are damaged in zebra fish and this is thought to act as a signal to white blood cells to converge on the site and initiate the healing process. When the genes required to produce hydrogen peroxide were disabled, white blood cells did not accumulate at the site of damage. Although the experiments were conducted on fish, they are genetically similar to humans and so this may also be applicable to humans. Asthma sufferers have higher levels of hydrogen peroxide in their lungs than healthy people and this could explain why asthma sufferers have inappropriate levels of white blood cells in their lungs .

6 . 4 . Domestic uses

- Diluted H_2O_2 (between 3 % and 12 %) is used to bleach human hair when mixed with ammonia, hence the phrase " peroxide blonde ". It is absorbed by skin upon contact and creates a local skin capillary embolism which appears as a temporary whitening of the skin. It is used to whiten bones that are to be put on display. The strength of a solution may be described as a percentage or volume, where 1 % hydrogen peroxide releases 3.3 volumes of oxygen during decomposition. Thus, a 3 % solution is equivalent to 10 volume and a 6 % solution to 20 volume, etc.
- 3 % H_2O_2 is used medically for cleaning wounds, removing dead tissue, and as an oral debriding agent. Peroxide stops slow (small vessel) wound bleeding/oozing, as well. Most over - the-counter peroxide solutions are not suitable for ingestion.
- 3 % H_2O_2 is effective at treating fresh (red) blood - stains in clothing and on other items. It must be applied to clothing before blood stains can be accidentally " set " with heated water. Cold water and soap are then used to remove the peroxide treated blood.

- The United States Food and Drug Administration (FDA) has classified hydrogen peroxide as a Low Regulatory Priority (LRP) drug for use in controlling fungus on fish and fish eggs.
- Some horticulturalists and users of hydroponics advocate the use of weak hydrogen peroxide solution (" Spanish water ") in watering solutions. Its spontaneous decomposition releases oxygen that enhances a plant's root development and helps to treat root rot (cellular root death due to lack of oxygen) and a variety of other pests. There is some peer-reviewed academic research to back up some of the claims.
- Laboratory tests conducted by fish culturists in recent years have demonstrated that common household hydrogen peroxide can be used safely to provide oxygen for small fish. Hydrogen peroxide releases oxygen by decomposition when it is exposed to catalysts such as manganese dioxide.
- Hydrogen peroxide is a strong oxidizer effective in controlling sulfide and organic related odors in wastewater collection and treatment systems. It is typically applied to a wastewater system where there is a retention time of 30 minutes to 5 hours before hydrogen sulfide is released. Hydrogen peroxide oxidizes the hydrogen sulfide and promotes bio - oxidation of organic odors. Hydrogen peroxide decomposes to oxygen and water, adding dissolved oxygen to the system thereby negating some Biochemical Oxygen Demand (BOD).
- Mixed with baking soda and a small amount of hand soap, hydrogen peroxide is effective at removing skunk odor. [26]
- If a dog has swallowed a harmful substance (e.g. rat poison, chocolate), small amounts of hydrogen peroxide can be given to induce vomiting.
- Hydrogen peroxide is used with phenyl oxalate ester and an appropriate dye in glow sticks as an oxidizing agent. It reacts with the ester to form an unstable CO_2 dimer which excites the dye to an excited state; the dye emits a photon (light) when it spontaneously relaxes back to the ground state.

6 . 5 . Use as propellant

H_2O_2 can be used either as a mono propellant (not mixed with fuel) or as the oxidizer component of a bipropellant rocket. Use as a monopropellant takes advantage of the decomposition of 70 – 98+ % concentration hydrogen peroxide into steam and oxygen. The propellant is pumped into a reaction chamber where a catalyst, usually a silver or platinum screen, triggers decomposition, producing steam at over 600 °C which is expelled through a nozzle, generating thrust. H_2O_2 monopropellant produces a maximum specific impulse (I_{sp}) of 161 s (1.6 kN·s / kg), which makes it a low-performance monopropellant. Peroxide generates much less thrust than hydrazine, but is not toxic. The Bell Rocket Belt used hydrogen peroxide mono propellant.

As a bipropellant H_2O_2 is decomposed to burn a fuel as an oxidizer. Specific impulses as high as 350 s (3.5 kN·s/kg) can be achieved, depending on the fuel. Peroxide used as an oxidizer gives a somewhat lower I_{sp} than liquid oxygen, but is dense, storable, noncryogenic and can be more easily used to drive gas turbines to give high pressures using an efficient *closed cycle*. It can also be used for regenerative cooling of rocket engines. Peroxide was used very successfully as an oxidizer in World - War - II German rockets (e.g. T - Stoff for the Me-163) , and for the low - cost British Black Knight and Black Arrow launchers.

In the 1940s and 1950s the Walter turbine used hydrogen peroxide for use in submarines while submerged; it was found to be too noisy and require too much maintenance compared to diesel - electric power systems. Some torpedoes used hydrogen peroxide as oxidizer or propellant, but this was dangerous and has been discontinued by most navies. Hydrogen peroxide leaks were blamed for the sinkings of HMS *Sidon* and the Russian submarine *Kursk*. It was discovered, for example, by the Japanese Navy in torpedo trials, that the concentration of H_2O_2 in right-angle bends in HTP pipework can often lead to explosions in submarines and torpedoes. SAAB Underwater Systems is manufacturing the Torpedo 2000. This torpedo, used by the Swedish navy, is powered by a piston engine propelled by HTP as an oxidizer and kerosene as a fuel in a bipropellant system .

While rarely used now as a monopropellant for large engines, small hydrogen peroxide attitude control thrusters are still in use on some satellites. They are easy to throttle, and safer to fuel and handle before launch than hydrazine thrusters. However, hydrazine is more often used in spacecraft because of its higher specific impulse and lower rate of decomposition.

Recently H_2O_2 / propylene has been proposed for an inexpensive single – stage – to - orbit (SSTO) vehicle. Its fuel tank would contain propylene with a H_2O_2 - filled bladder floating in it. This combination offers 15 % superior I_{sp} to O2 / RP4 (a kerosene used as rocket propellant), does not need turbines or cryogenic storage or hardware, and greatly reduces the cost of the booster. The potential of this and other alternative systems is discussed in some detail at Dunn Engineering.

6 . 6 . Therapeutic use

Hydrogen peroxide is *generally recognized as safe* (GRAS) as an antimicrobial agent, an oxidizing agent and for other purposes by the FDA .

Hydrogen peroxide has been used as an antiseptic and anti-bacterial agent for many years due to its oxidizing effect. While its use has decreased in recent years with the popularity of readily-available over the counter products, it is still used by many hospitals, doctors and dentists.

- Like many oxidative antiseptics, hydrogen peroxide causes mild damage to tissue in open wounds, but it also is effective at rapidly stopping capillary bleeding (slow blood oozing from small vessels in abrasions), and is sometimes used sparingly for this purpose, as well as cleaning.
- Hydrogen peroxide can be used as a toothpaste when mixed with correct quantities of baking soda and salt.

- Hydrogen peroxide and benzoyl peroxide are sometimes used to treat acne.
- Hydrogen peroxide is used as an emetic in veterinary practice.

Alternative uses

- The American Cancer Society states that "there is no scientific evidence that hydrogen peroxide is a safe, effective or useful cancer treatment", and advises cancer patients to "remain in the care of qualified doctors who use proven methods of treatment and approved clinical trials of promising new treatments."
- Another controversial alternative medical procedure is inhalation of hydrogen peroxide at a concentration of about 1%. Internal use of high concentration hydrogen peroxide has a history of causing fatal blood disorders, and its recent use as a therapeutic treatment has been linked to several deaths .

7 . Safety

Regulations vary, but low concentrations, such as 3 %, are widely available and legal to buy for medical use. Higher concentrations may be considered hazardous and are typically accompanied by a Material Safety Data Sheet (MSDS). In high concentrations, hydrogen peroxide is an aggressive oxidizer and will corrode many materials, including human skin. In the presence of a reducing agent, high concentrations of H_2O_2 will react violently.

Hydrogen peroxide should be stored in a cool, dry, well - ventilated area and away from any flammable or combustible substances . It should be stored in a container composed of non-reactive materials such as stainless steel or glass (other materials including some plastics and aluminium alloys may also be suitable) . Because it breaks down quickly when exposed to light, it should be stored in an opaque container, and pharmaceutical formulations typically come in brown bottles that filter out light .

Hydrogen peroxide, either in pure or diluted form, can pose several risks:

- Above roughly 70 % concentrations, hydrogen peroxide can give off vapor that can detonate above 70 °C at normal atmospheric pressure. This can then cause a boiling liquid expanding vapor explosion (BLEVE) of the remaining liquid. Distillation of hydrogen peroxide at normal pressures is thus highly dangerous.
- Hydrogen peroxide vapors can form sensitive contact explosives with hydrocarbons such as greases. Hazardous reactions ranging from ignition to explosion have been reported with alcohols, ketones, carboxylic acids (particularly acetic acid), amines and phosphorus.
- Concentrated hydrogen peroxide, if spilled on clothing (or other flammable materials) , will preferentially evaporate water until the concentration reaches sufficient strength, at which point the material may spontaneously ignite.
- Concentrated hydrogen peroxide (> 50 %) is corrosive, and even domestic - strength solutions can cause irritation to the eyes, mucous membranes and skin . Swallowing hydrogen peroxide solutions is particularly dangerous, as decomposition in the stomach releases large quantities of gas (10 times the volume of a 3 % solution) leading to internal bleeding. Inhaling over 10 % can cause severe pulmonary irritation.
- Low concentrations of hydrogen peroxide, on the order of 3% or less, will chemically bleach many types of clothing to a pinkish hue. Caution should be exercised when using common products that may contain hydrogen peroxide, such as facial cleaner or contact lens solution, which easily splatter upon other surfaces.
- Large oral doses of hydrogen peroxide at a 3 % concentration may cause " irritation and blistering to the mouth, (which is known as Black Hairy Tongue) throat, and abdomen ", as well as " abdominal pain, vomiting, and diarrhea ".
- Hydrogen peroxide has a significant vapor pressure (1.2 kPa at 50 ^{o}C and exposure to the vapor is potentially

hazardous. Hydrogen peroxide vapor is a primary irritant, primarily affecting the eyes and respiratory system and the NIOSH Immediately dangerous to life and health limit (IDLH) is only 75 ppm.

- Long term exposure to low ppm concentrations is also hazardous and can result in permanent lung damage and OSHAO ccupational Safety and Health Administration has established a permissible exposure limit of 1.0 ppm calculated as an eight hour time weighted average (29 CFR 1910.1000, Table Z – 1) and hydrogen peroxide has also been classified by the ACGIH American Conference of Industrial Hygienists (ACGIH) as a " known animal carcinogen, with unknown relevance on humans.[2008 Threshold Limit Values for Chemical Substances and Physical Agents & Biological Exposure Indices, ACGIH] In applications where high concentrations of hydrogen peroxide are used, suitable personal protective equipment should be worn and it is prudent in situations where the vapor is likely to be generated, such as hydrogen peroxide gas or vapor sterilization, to ensure that there is adequate ventilation and the vapor concentration monitored with a continuous gas monitor for hydrogen peroxide. Continuous gas monitors for hydrogen peroxide are available from several suppliers. Further information on the hazards of hydrogen peroxide is available from OSHA Occupational Safety and Health Guideline for Hydrogen Peroxide and from the ATSDR. Agency for Toxic Substances and Disease Registry
- Vitiligo is an acquired skin disorder with the loss of native skin pigment, which affects about 0.5-1% of the world population. Recent studies have discovered increased H_2O_2 levels in the epidermis and in blood are one of many hallmarks of this disease.

7 . 1 . Historical incidents

- Several people received minor injuries after a hydrogen peroxide spill on board Northwest Airlines flight 957 from Orlando to Memphis on October 28, 1998 and subsequent fire on Northwest Airlines flight 7.

- During the Second World War, Doctors in Nazi concentration camps experimented with the use of hydrogen peroxide injections in the killing of human subjects.
- Hydrogen peroxide was said to be one of the ingredients in the bombs which failed to explode in the 21 July 2005 London bombings.
- The Russian submarine K - 141 Kursk sailed out to sea to perform an exercise of firing dummy torpedoes at the Pyotr Velikiy, a Kirov class battlecruiser. On August 12, 2000 at 11:28 local time (07:28 UTC), there was an explosion while preparing to fire the torpedoes. The only credible report to date is that this was due to the failure and explosion of one of the Kursk's hydrogen peroxide - fuelled torpedoes. It is believed that HTP, a form of highly concentrated hydrogen peroxide used as propellant for the torpedo, seeped through rust in the torpedo casing. A similar incident was responsible for the loss of HMS Sidon in 1955.

Deuterium

Contents

1 . Introduction :

Deuterium, also called **heavy hydrogen**, is a stable isotope of hydrogen with a natural abundance in the oceans of Earth of approximately one atom in 6,500 of hydrogen (~154 ppm). Deuterium thus accounts for approximately 0.015 % (alternately, on a weight basis : 0.031 %) of all naturally occurring hydrogen in the oceans on

Earth . Deuterium abundance on Jupiter is about 2.25×10^{-5} (roughly 22 atoms in a million, or 15 % of the terrestrial deuterium - to - hydrogen ratio) ; these ratios presumably reflect the early solar nebula ratios, and those after the Big Bang. However, other sources suggest a much higher abundance of e.g. 6×10^{-4} (6 atoms in 10,000 or 0.06% atom basis) . There is little deuterium in the interior of the Sun, since thermonuclear reactions destroy it. However, it continues to persist in the outer solar atmosphere at roughly the same concentration as in Jupiter.

The nucleus of deuterium, called a **deuteron**, contains one proton and one neutron, whereas the far more common hydrogen nucleus contains no neutrons. The isotope name is formed from the Greek *deuteros* meaning " second ", to denote the two particles composing the nucleus.

Name, symbol	deuterium, ^{2}H or D
Neutrons	1
Protons	1
Nuclide Data	
Natural abundance	0.015 %
Half - life	Stable
Isotope Mass	2.01410178 u
Spin	1^{+}
Excess energy	13,135.720 ± 0.001 keV
Binding energy	2,224.52 ± 0.20 keV

2 . Differences between deuterium and common hydrogen (protium)

2 . 1 . Chemical symbol

Deuterium is frequently represented by the chemical symbol D. Since it is an isotope of hydrogen with mass number 2, it is also represented by ^{2}H. IUPAC allows both D and ^{2}H, although ^{2}H is preferred.[4] The reason deuterium has a distinct chemical symbol may be its large mass difference with protium (^{1}H) ; deuterium has a mass of 2.014102 u, compared to the mean hydrogen atomic weight of 1.007947 u, and protium's mass of 1.007825 u. The isotope weight ratios within other chemical elements are largely insignificant in this regard, explaining the lack of unique isotope symbols elsewhere .

2 . 2 . Natural abundance

Deuterium occurs in trace amounts naturally as deuterium gas, written $^2H_2$ or D_2, but most natural occurrence in the universe is bonded with a typical ^{1}H atom, a gas called hydrogen deuteride (HD or $^1H\ ^2H$) .

The existence of deuterium on Earth, elsewhere in the solar system (as confirmed by planetary probes), and in the spectra of stars, is an important datum in cosmology. Stellar fusion destroys deuterium, and there are no known natural processes other than the Big Bang nucleosynthesis, which might have produced deuterium at anything close to the observed natural abundance of deuterium (deuterium is produced by the rare cluster decay, and occasional absorption of naturally - occuring neutrons by light hydrogen, but these are trivial sources). The natural deuterium abundance seems to be a very similar fraction of hydrogen, wherever hydrogen is found. Thus, the existence of deuterium at a low but constant fraction in all hydrogen, is one of the arguments in favor of the Big Bang theory over the steady state theory of the universe. It is estimated that the abundances of deuterium have not evolved significantly since their production about 13.7 billion years ago.

The world's leading " producer " of deuterium (technically, merely enricher or concentrator of deuterium) was Canada, until 1997 when the last plant was shut down . Canada uses heavy water as a neutron moderator for the operation of the CANDU reactor design. India is now probably the world's largest concentrator of heavy water, also used in nuclear power reactors.

3 . Physical properties

The physical properties of deuterium compounds can exhibit significant kinetic isotope effects and other physical and chemical property differences from the hydrogen analogs; for example, D_2O is more viscous than H_2O. Chemically, deuterium behaves similarly to ordinary hydrogen, but there are differences in bond energy and length for compounds of heavy hydrogen isotopes which are larger than the isotopic differences in any other element. Bonds involving deuterium and tritium are somewhat stronger than the corresponding bonds in hydrogen, and these differences are enough to make significant changes in biological reactions .

Deuterium can replace the normal hydrogen in water molecules to form heavy water (D_2O), which is about 10.6 % denser than normal water (enough that ice made from it sinks in ordinary water). Heavy water is slightly toxic in eukaryotic animals, with 25 % substitution of the body water causing cell division problems and sterility, and 50% substitution causing death by cytotoxic syndrome (bone marrow failure and gastrointestinal lining failure). Prokaryotic organisms, however, can survive and grow in pure heavy water (though they grow more slowly). Consumption of heavy water would not pose a health threat to humans unless very large quantities (in excess of 10 liters) were consumed over many days. Small doses of heavy water (a few grams in humans, containing an amount of deuterium comparable to that normally present in the body) are routinely used as harmless metabolic tracers in humans and animals.

4 . Quantum properties

The deuteron has spin +1 and is thus a boson. The NMR frequency of deuterium is significantly different from common light hydrogen. Infrared spectroscopy also easily differentiates many deuterated compounds, due to the large difference in IR absorption frequency seen in the vibration of a chemical bond containing deuterium, versus light hydrogen. The two stable isotopes of hydrogen can also be distinguished by using mass spectrometry.

5 . Nuclear properties

Deuterium is one of only four stable nuclides with an odd number of protons and odd number of neutrons. (^{2}H, ^{6}Li, ^{10}B, ^{14}N ; also, the long - lived radioactive nuclides ^{40}K, ^{50}V, ^{138}La, ^{180m}Ta occur naturally.) Most odd-odd nuclei are unstable with respect to beta decay, because the decay products are even - even, and are therefore more strongly bound, due to nuclear pairing effects. Deuterium, however, benefits from having its proton and neutron coupled to a spin-1 state, which gives a stronger nuclear attraction; the corresponding spin-1 state does not exist in the two-neutron or two - proton system, due to the Pauli exclusion principle which would require one or the other identical particle with the same spin to have some other different quantum number, such as orbital angular momentum. But orbital angular momentum of either particle gives a lower binding energy for the system, primarily due to increasing distance of the particles in the steep gradient of the nuclear force. In both cases, this causes the diproton and dineutron nucleus to be unstable.

The proton and neutron making up deuterium can be dissociated through neutral current interactions with neutrinos. The cross section for this interaction is comparatively large, and deuterium was successfully used as a neutrino target in the Sudbury Neutrino Observatory experiment.

5 . 1 . Deuterium as an isospin singlet

Due to the similarity in mass and nuclear properties between the proton and neutron, they are sometimes considered as two symmetric types of the same object, a nucleon. While only the proton has an electric charge, this is often negligible due of the weakness of the electromagnetic interaction relative to the strong nuclear interaction. The symmetry relating the proton and neutron is known as isospin and denoted I (or some times T).

Isospin is an SU (2) symmetry, like ordinary spin, so is completely analogous to it. The proton and neutron form an isospin doublet, with a "down" state (↓) being a neutron, and an "up" state (↑) being a proton.

A pair of nucleons can either be in an antisymmetric state of isospin called singlet, or in a symmetric state called triplet. In terms of the "down" state and "up" state, the singlet is

This is a nucleus with one proton and one neutron, i.e. a deuterium nucleus. The triplet is *****

and thus consists of three types of nuclei, which are supposed to be symmetric: a deuterium nucleus (actually a highly excited state of it), a nucleus with two protons, and a nucleus with two neutrons. The latter two nuclei are not stable or nearly stable, and therefore so is this type of deuterium (meaning that it is indeed a highly excited state of deuterium).

5 . 2 . Approximated wavefunction of the deuteron

The total wavefunction of both the proton and neutron must be antisymmetric, because they are both fermions. Apart from their isospin, the two nucleons also have spin and spatial distributions of their wavefunction. The latter is symmetric if the deuteron is symmetric under parity (i.e. have an "even" or "positive" parity) , and antisymmetric if the deuteron is antisymmetric under parity (i.e. have an "odd" or "negative" parity). The parity is fully determined by the total orbital angular momentum of the two nucleons: if it is even then the parity is even (positive), and if it is odd then the parity is odd (negative).

The deuteron, being an isospin singlet, is antisymmetric under nucleons exchange due to isospin, and therefore must be symmetric under the double exchange of their spin and location. Therefore it can be in either of the following two different states:

- Symmetric spin and symmetric under parity. In this case, the exchange of the two nucleons will multiply the deuterium wavefunction by (-1) from isospin exchange, (+1) from spin exchange and (+1) from parity (location exchange), for a total of (-1) as needed for antisymmetry.

- Antisymmetric spin and antisymmetric under parity. In this case, the exchange of the two nucleons will multiply the deuterium wavefunction by (-1) from isospin exchange, (-1) from spin exchange and (-1) from parity (location exchange), again for a total of (-1) as needed for antisymmetry.

In the first case the deuteron is a spin triplet, so that its total spin *s* is 1. It also has an even parity and therefore even orbital angular momentum *l* ; The lower its orbital angular momentum, the lower its energy. Therefore the lowest possible energy state has *s* = 1, *l* = 0.

In the second case the deuteron is a spin singlet, so that its total spin *s* is 0. It also has an odd parity and therefore odd orbital angular momentum *l* . There fore the lowest possible energy state has *s* = 0 , *l* = 1.

Since *s* = 1 gives a stronger nuclear attraction, the deuterium ground state is in the *s* =1, {{{1}}} state.

The same considerations lead to the possible states of an isospin triplet having *s* = 0, *l* = even or *s* = 1 , *l* = odd. Thus the state of lowest energy has *s* = 1 , *l* = 1, higher than that of the isospin singlet.

The analysis just given is in fact only approximate, both because isospin is not an exact symmetry, and more importantly because the strong nuclear interaction between the two nucleons is related to angular momentum in spin - orbit interaction that mixes different *s* and *l* states. That is, *s* and *l* are not constant in time (they do not commute with the Hamiltonian), and over time a state such as *s* = 1, *l* = 0 may become a state of *s* = 1, *l* = 2. Parity is still constant in time so these do not mix with odd *l* states (such as *s* = 0, *l* = 1). Therefore the quantum state of the deuterium is a superposition (a linear combination) of the *s* = 1, *l* = 0 state and the *s* = 1, *l* = 2 state, even though the first component is much bigger. Since the total angular momentum *j* is also a good quantum number (it is a constant in time), both components must have the same *j*, and therefore *j* = 1. This is the total spin of the deuterium nucleus.

To summarize, the deuterium nucleus is antisymmetric in terms of isospin, and has spin 1 and even (+1) parity. The relative angular momentum of its nucleons *l* is not well defined, and the deuteron is a superposition of mostly $l = 0$ with some $l = 2$.

5 . 2 . Magnetic and electric multipoles

In order to find theoretically the deuterium magnetic dipole moment μ, one uses the formula for a nuclear magnetic moment with $g^{(l)}$ and $g^{(s)}$ are g - factors of the nucleons.

Since the proton and neutron have different values for $g^{(l)}$ and $g^{(s)}$, one must separate their contributions. Each gets half of the deuterium orbital angular momentum and spin . One arrives at where subscripts p and n stand for the proton and neutron, and $g^{(l)}_n = 0$.

By using the same identities as here and using the value $g^{(l)}_p = 1\ \mu_N$, we arrive at the following result, in nuclear magneton units

For the $s = 1$, $l = 0$ state ($j = 1$), we get

For the $s = 1$, $l = 2$ state ($j = 1$), we get

The measured value of the deuterium magnetic dipole moment, is 0.857 μ_N. This suggests that the state of the deuterium is indeed only approximately $s = 1$, $l = 0$ state, and is actually a linear combination of (mostly) this state with $s = 1$, $l = 2$ state.

The electric dipole is zero as usual.

The measured electric quadropole of the deuterium is 0.2859 [[|elementary charge|e]]·fm^2. While the order of magnitude is reasonable, since the deuterium radius is of order of 1 femtometer (see below) and its electric charge is e, the above model does not suffice for its computation. More specifically, the electric quadrupole does not get a contribution from the $l = 0$ state (which is the dominant one) and does get a contribution from a term mixing the $l = 0$ and the $l = 2$ states, because the electric quadrupole operator does not commute with angular momentum. The latter contribution is dominant in the absence of a pure $l = 0$ contribution, but cannot be calculated without knowing the exact spatial form of the nucleons wavefunction inside the deuterium.

Higher magnetic and electric multipole moments cannot be calculated by the above model, for similar reasons.

5 . 4 . Deuterium radius

The square root of the average squared radius of the deuterium, measured experimentally, is

6 . Applications

Emission spectrum of an ultraviolet deuterium arc lamp.

Deuterium has a number of commercial and scientific uses. These include:

6 . 1 . Deuterium in nuclear reactors

Deuterium is useful in nuclear fusion reactions, especially in combination with tritium, because of the large reaction rate (or nuclear cross section) and high energy yield of the D –T reaction. There is an even higher-yield D – ^{3}He fusion reaction, though the breakeven point of D – ^{3}He is higher than that of most other fusion reactions; together with the scarcity of ^{3}He, this makes it implausible as a practical power source until at least D –T and D – D fusion reactions have been performed on a commercial scale.

Deuterium is used in heavy water moderated fission reactors, usually as liquid D_2O, to slow neutrons without high neutron absorption of ordinary hydrogen.

6 . 2 . Deuterium NMR spectroscopy

Deuterium NMR spectra are especially informative in the solid state because of its relatively small quadrupole moment in comparison with those of bigger quadrupolar nuclei such as Chloride-35, for example.

6 . 3 . A stable isotope tracer

In chemistry, biochemistry and environmental sciences, deuterium is used as a non - radioactive, stable isotopic tracer. In chemical reactions and metabolic pathways, deuterium behaves similarly to ordinary hydrogen, but it can be distinguished from ordinary hydrogen by its mass, using mass spectrometry or infrared spectrometry. Deuterium can be detected by femtosecond infrared spectroscopy, since the mass difference drastically affects the frequency of molecular vibrations; deuterium - carbon bond vibrations are found in locations free of other signals.

Measurements of small variations in the natural abundances of deuterium, along with those of the stable heavy oxygen isotopes ^{17}O and ^{18}O, are of importance in hydrology, to trace the geographic origin of Earth's waters. The heavy isotopes of hydrogen and oxygen in rainwater (so - called meteoric water) are enriched as a function of the environmental temperature of the region in which the precipitation falls (and thus enrichment is related to mean latitude). The relative enrichment of the heavy isotopes in rainwater (as referenced to mean ocean water), when plotted against temperature falls predictably along a line called the global meteoric water line (GMWL). This plot allows samples of precipitation-originated water to be identified along with general information about the climate in which it originated. Evaporative and other processes in bodies of water, and also ground water processes, also differentially alter the ratios of heavy hydrogen and oxygen isotopes in fresh and salt waters, in characteristic and often regionally - distinctive ways.

6 . 4 . Neutron scattering scattering contrast properties

Neutron scattering techniques particularly profit from availability of deuterated samples: The H and D cross sections are very distinct and different in sign, which allows contrast variation in such experiments. Further, a nuisance problem of ordinary hydrogen is its large incoherent neutron cross section, which is nil for D and delivers much clearer signals in deuterated samples. Hydrogen occurs in all materials of organic chemistry and life science, but cannot be seen by X-ray diffraction methods. Hydrogen can be seen by neutron diffraction and scattering, which makes neutron scattering, together with a modern deuteration facility, indispensable for many studies of macromolecules in biology and many other areas.

6 . 5 . Nuclear resonance spectroscopy

Deuterium is useful in hydrogen nuclear magnetic resonance spectroscopy (proton NMR). NMR ordinarily requires compounds of interest to be analyzed as dissolved in solution. Because of deuterium's nuclear spin properties which differ from the light hydrogen usually present in organic molecules, NMR spectra of hydrogen/protium are highly differentiable from that of deuterium, and in practice deuterium is not "seen" by an NMR instrument tuned to light-hydrogen. Deuterated solvents (including heavy water, but also compounds like deuterated chloroform, $CDCl_3$) are therefore routinely used in NMR spectroscopy, in order to allow only the light-hydrogen spectra of the compound of interest to be measured, without solvent-signal interference.

7 . History

7 . 1 . Lighter element isotopes suspected

The existence of nonradioactive isotopes of lighter elements had been suspected in studies of neon as early as 1913, and proven by mass spectroscopy of light elements in 1920. The prevailing theory at the time, however, was that the isotopes were due to the existence of differing numbers of "nuclear electrons" in different atoms of an element. It was expected that hydrogen, with a measured average atomic mass very close to 1 **u**, and a nucleus thought to be composed of a single proton (a known particle), could not contain nuclear electrons, and thus could have no heavy isotopes.

7 . 2 . Deuterium predicted and finally detected

Deuterium was predicted in 1926 by Walter Russell, using his "spiral" periodic table. It was first detected spectroscopically in late 1931 by Harold Urey, a chemist at Columbia University. Urey's collaborator, Ferdinand Brickwedde, distilled five liters of cryogenically-produced liquid hydrogen to 1 mL of liquid, using the low-temperature physics laboratory that had recently been established at the National Bureau of Standards in Washington, D.C. (now the National Institute of Standards and Technology) . This concentrated the fraction of the mass - 2 isotope of hydrogen to a degree that made its spectroscopic identification unambiguous; Urey called the isotope "deuterium" from the Greek and Latin words for "two". The amount inferred for normal abundance of this heavy isotope was so small (only about 1 atom in 6400 hydrogen atoms in ocean water) that it had not noticeably affected previous measurements of (average) hydrogen atomic mass. Urey was also able to concentrate water to show partial enrichment of deuterium. Gilbert Newton Lewis prepared the first samples of pure heavy water in 1933. The discovery of deuterium, coming before the discovery of the neutron in 1932, was an experimental shock to theory, and after the neutron was reported, deuterium won Urey the Nobel Prize in chemistry in 1934.

7 . 3 . " Heavy water " experiments in World War II

Shortly before the war, Hans von Halban and Lew Kowarski moved their research on neutron moderation from France to England, smuggling the entire global supply of heavy water (which had been made in Norway) across in twenty-six steel drums.

During World War II, Nazi Germany was known to be conducting experiments using heavy water as moderator for a nuclear reactor design. (Heavy water is water in which the hydrogen is deuterium.) Such experiments were a source of concern because they might allow them to produce plutonium for an atomic bomb. Ultimately it led to the Allied operation called the "Norwegian heavy water sabotage," the purpose of which was to destroy the Vemork deuterium production/enrichment facility in Norway. At the time this was considered important to the potential progress of the war.

After World War II ended, the Allies discovered that Germany was not putting as much serious effort into the program as had been previously thought.The Germans had completed only a small, partlybuilt experimental reactor (which had been hidden away). By the end of the war, the Germans did not even have a fifth of the amount of heavy water needed to run the reactor, partially due to the Norwegian heavy water sabotage operation. However, even had the Germans succeeded in getting a reactor operational (as the U.S. did with a graphite reactor in late 1942) , they would still have been at least several years away from development of an atomic bomb with maximal effort. The engineering process, even with maximal effort and funding, required about two and a half years (from first critical reactor to bomb) in both the U.S. and U.S.S.R, for example.

7 . 4 . Name

Urey called the molecule "deuterium", from the Greek deuteros (second), and the nucleus to be called "deuteron" or "deuton". The molecules were traditionally given the name that its discoverer decided, but some British chemists, like Ernest Rutherford, wanted the molecule to be called "diplogen", from the Greek diploos (double), and the nucleus to be called diplon. The British magazine Nature also published a letter where only the denomination "diplogen" was used, perhaps annunciating that British could prefer that name over the name given by its discoverer. Urey and his two co-discoverers sent a letter to Nature saying that they had already considered that name and they had rejected it because "The compound N H1 H2 / 2 would be called di - diplogen mono-hydrogen nitride", which would repeat the syllable "di." They also said that the British seemed to object on the basis that "neutron" and "deuton" could be confused with each other, and he points out that American workers were using the terms and they didn't seem to be having any such confusion.[3]

8 . Data

- Density: 0.180 kg / m^3 at STP (0 °C, 101.325 kPa).
- Atomic weight: 2.01355321270 u.
- Mean abundance in ocean water (see VSMOW) about 0.0156 % of H atoms = 1 / 6400 H atoms.

Data at approximately 18 K for D_2 (triple point) :

- Density:
    - Liquid : 162.4 kg/m^3
    - Gas : 0.452 kg/m^3
- Viscosity : 12.6 µPa·s at 300 K (gas phase)
- Specific heat capacity at constant pressure c_p:
    - Solid : 2,950 J / (kg · K)
    - Gas: 5,200 J / (kg· K)

8 . Anti - deuterium

An **antideuteron** is the antiparticle of the nucleus of deuterium, consisting of an antiproton and an antineutron. The antideuteron was first produced in 1965 at the Proton Synchrotron at CERN and the Alternating Gradient Synchrotron at Brookhaven National Laboratory. A complete atom, with a positron orbiting the nucleus, would be called *antideuterium*, but as of 2005 antideuterium has not yet been created. The proposed symbol for antideuterium is D, that is, D with an overbar.

10 . Pycnodeuterium

Deuterium atoms can be absorbed into a palladium (Pd) lattice. They are effectively solidified as an ultrahigh density deuterium lump (*Pycnodeuterium*) inside each octahedral space within the unit cell of the palladium host lattice. Some believe it may be possible to use this as a nuclear fuel in cold fusion. However, cold fusion by this mechanism has not been generally accepted by the scientific community.

Heavy water

Contents

1 . Introduction :

Heavy water is water that contains a higher proportion than normal of the isotope deuterium, as **deuterium oxide**, D_2O or ^2H_2O , or as **deuterium protium oxide**, HDO or $^1H\,^2H\,O$. Its physical and chemical properties are somewhat similar to those of water, H_2O.

Heavy water may contain as much as 100 % $D_2 O$, and usually the term refers to water that is highly enriched in deuterium. The isotopic substitution with deuterium alters the bond energy of the hydrogen-oxygen bond in water, altering the physical, chemical, and especially biological properties of the pure or highly - enriched substance to a larger degree than is found in most isotope - substituted chemical compounds.

Relatively pure heavy water was produced in 1933, soon after the discovery of deuterium, the stable heavy isotope of hydrogen. With the discovery of nuclear fission in late 1938 and the need for a neutron moderator which captured few neutrons, heavy water soon achieved importance in relation to early nuclear programs during World War II. Due in part to German reliance on scarce heavy water for reactor research in this war, Germany did not succeed in producing a functioning reactor during World War II. Since this war, heavy water has played a part in a number of reactor designs, both in designs for power and for nuclear weapon-making. Reactors which use enriched uranium, however, are able to use normal “ light - water ” for neutron moderation, and remain the most common type of reactor in use today.

Heavy water itself is not radioactive, and has physical properties similar to water save for being about 11 % more dense. However, as commercially made, heavy water contains whatever tritium was present in the water from which it was isolated. When the water in eukaryotic organisms is replaced by more than about 25 to 50 % heavy water, they experience toxicity due to interference by the deuterium with the mitotic apparatus of these cells. Higher organisms, including mammals, if given only heavy water, soon become ill and die at the point that about half their body water has been replaced. Bacteria, however, are able to grow slowly in pure heavy water.

Small concentrations of heavy water are nontoxic. The adult human body naturally contains deuterium equivalent to the amount in about 5 grams of heavy water, and comparable doses of heavy water are still used as safe non - radioactive tracers for metabolic experiments in humans and other animals.

Other Names	Water - d_2 Heavy water Dideuterium monoxide
Molecular Formula	D_2O
Molar Mass	20.04 g / mol
Appearance	transparent, colorless liquid
Density	1.1056 g / mL , liquid (20° C) 1.0177 g / cm^3, solid (at m.p)
Melting point	3.82 °C
Boiling point	101.4 °C
Viscosity	0.00125 Pa·s at 20 °C
Dipole moment	1.87 D

2 . Other meanings

2 . 1 . Semiheavy water

Semi heavy water, HDO, exists whenever there is water with hydrogen - 1 (or protium) and deuterium present in the mixture. This is because hydrogen atoms (hydrogen - 1 and deuterium) are rapidly exchanged between water molecules. Water containing 50 % H and 50 % D in its hydrogen actually contains about 50 % HDO and 25 % each of H_2O and D_2O , in dynamic equilibrium. Semiheavy water, HDO, occurs naturally in regular water at a proportion of about 1 molecule in 3,200 (each hydrogen has a probability of 1 in 6,400 of being D). Heavy water, D_2O , by comparison, occurs naturally at a proportion of about 1 molecule in 41 million (i.e., 1 in $6{,}400^2$) . This makes semiheavy water actually far more prevalent than 'normal' heavy water.

2 . 2 . Heavy - Oxygen Water

A common type of heavy - oxygen water $H_2{}^{18}O$ is available commercially for use as a non - radioactive isotopic tracer . and qualifies as "heavy water" insofar as having a higher density than normal water (in this case, similar density to deuterium oxide). At higher expense (due to the greater difficulty in separation of O-17, a less common heavy isotope of oxygen), water is available in which the oxygen is enriched to varying degrees with ^{17}O. However, these types of heavy-isotope water are rarely referred to as "heavy water", as they do not contain the deuterium which gives D_2O its characteristically different nuclear and biological properties. Heavy - oxygen waters with normal hydrogen, for example, would not be expected to show any toxicity whatsoever .

3 . Physical properties (with comparison to light water) :

Property	D_2O (Heavy water)	H_2O (Light water)
Freezing point (°C)	3.82	0.0
Boiling point (°C)	101.4	100.0
Density (at 20°C , g / mL)	1.1056	0.9982
Temp. of maximum density	11.6 (° C)	4.0 (° C)
Viscosity (at 20°C, mPa·s)	1.25	1.005
Surface tension (at 25°C, µJ)	7.193	7.197
Heat of fusion (cal / mol)	1,515	1,436
Heat of vaporisation (cal / mol)	10,864	10,515
pH (at 25°C)	7.41	7.00

No physical properties are listed for "pure" semi - heavy water, because it cannot be isolated in bulk quantities. In the liquid state, a few water molecules are always in an ionised state, which means the hydrogen atoms can exchange among different oxygen atoms. A sample of hypothetical "pure" semi - heavy water would rapidly transform into a dynamic mixture of 25 % light water, 25 % heavy water, and 50 % semi - heavy water.

Physical properties obvious by inspection :

Heavy water is 10.6 % denser than ordinary water, a difference which is difficult to notice in a sample of it (although it looks like water, it reportedly tastes slightly sweet). One of the few ways to demonstrate heavy water's physically different properties without equipment, is to freeze a sample and drop it into normal water. Ice made from heavy water *sinks* in normal water. If the normal water is ice - cold this phenomenon may be observed long enough for a good demonstration, since heavy-water ice has a slightly higher melting-temperature (3.8 °C) than normal ice, and thus holds up very well in ice - cold normal water.

4 . History

Harold Urey discovered the isotope deuterium in 1931 and was later able to concentrate it in water. Urey's mentor Gilbert Newton Lewis isolated the first sample of pure heavy water by electrolysis in 1933. George de Hevesy and Hoffer used heavy water in 1934 in one of the first biological tracer experiments, to estimate the rate of turnover of water in the human body. The history of large-quantity production and use of heavy water in early nuclear experiments is given below.[5]

5 . Effect on biological systems

Heavy isotopes of chemical elements have slightly different chemical behaviors, but for most elements the differences in chemical behavior between isotopes are far too small to use, or even detect. For hydrogen, however, this is not true. The larger chemical isotope-effects seen with deuterium and tritium manifest because bond energies in chemistry are determined in quantum mechanics by equations in which the quantity of reduced mass of the nucleus and electrons appears. This quantity is altered in heavy-hydrogen compounds (of which deuterium oxide is the most common and familiar) more than for heavy - isotope substitution in other chemical elements. This isotope effect of heavy hydrogen is magnified further in biological systems, which are very sensitive to small changes in the solvent properties of water.

Heavy water is the only known chemical substance that affects the period of circadian oscillations, consistently increasing them. The effect is seen in unicellular organisms, green plants, isopods, insects, birds, mice, and hamsters. The mechanism is unknown.

To perform their tasks, enzymes rely on their finely tuned networks of hydrogen bonds, both in the active center with their substrates, and outside the active center, to stabilize their tertiary structures. As a hydrogen bond with deuterium is slightly stronger than one involving ordinary hydrogen, in a highly deuterated environment, some normal reactions in cells are disrupted.

Particularly hard - hit by heavy water are the delicate assemblies of mitotic spindle formation necessary for cell division in eukaryotes. Plants stop growing and seeds do not germinate when given only heavy water, because heavy water stops eukaryotic cell division.

It has been proposed that low doses of heavy water can slow the aging process by helping the body resist oxidative damage via the isotope effect. A team at the Institute for the Biology of Ageing, located in Moscow, conducted an experiment to determine the effect of heavy water on longevity using fruit flies and found that while large amounts were deadly, smaller quantities increased lifespans by up to 30 % .

5 . 1 . Effect on animals

Experiments in mice, rats, and dogs have shown that a degree of 25% deuteration causes (some times irreversible) sterility, because neither gametes nor zygotes can develop. High concentrations of heavy water (90 %) rapidly kill fish, tadpoles, flatworms, and drosophila. Mammals, such as rats, given heavy water to drink die after a week, at a time when their body water approaches about 50% deuteration. The mode of death appears to be the same as that in cytotoxic poisoning (such as chemotherapy) or in acute radiation syndrome (though deuterium is not radioactive), and is due to deuterium's action in generally inhibiting cell division. It is more toxic to malignant cells than normal cells but the concentrations needed are too high for regular use. As in chemotherapy, deuterium - poisoned mammals die of a failure of bone marrow (bleeding and infection) and intestinal-barrier functions (diarrhea and fluid loss) .

Notwithstanding the problems of plants and animals in living with too much deuterium, prokaryotic organisms such as bacteria, which do not have the mitotic problems induced by deuterium, may be grown and propagated in fully deuterated conditions, resulting in replacement of all hydrogen atoms in the bacterial proteins and DNA with the deuterium isotope.[9] Full replacement with heavy atom isotopes can be accomplished in higher organisms with other non-radioactive heavy isotopes (such as carbon - 13, nitrogen - 15, and oxygen - 18) , but this cannot be done for the stable heavy isotope of hydrogen . Deuterium oxide is used to enhance boron neutron capture therapy, but this effect does not rely on the biological effects of deuterium per se, but instead on deuterium's ability to moderate (slow) neutrons without capturing them.

5 . 2 . Toxicity in humans

Because it would take a very large amount of heavy water to replace 25 % to 50 % of a human being's body water (which in turn is 70 % of body weight) with heavy water, accidental or intentional poisoning with heavy water is unlikely to the point of practical disregard. For a poisoning, large amounts of heavy water would need to be ingested without significant normal water intake for many days to produce any noticeable toxic effects (although in a few tests, volunteers drinking large amounts of heavy water have reported dizziness, a possible effect of density changes in the fluid in the inner ear[*citation needed*]). For example, a 70 kg human containing 50 kg of water and drinking 3 litres of pure heavy water per day, would take almost 5 days to reach 25% deuteration and about 11 days to approach 50% deuteration. Thus, it would take a week of drinking nothing but pure heavy water for a human to begin to feel ill, and 10 days to 2 weeks (depending on water intake) for severe poisoning and death. In the highly unlikely event that a human were to receive a toxic dose of heavy water, the treatment would involve the use of intravenous water replacement (due to possible intestinal dysfunction and problems with absorption of fluids). This would be done via 0.9 % (normal physiologic) saline solution with other salts as needed, perhaps in conjunction with diuretics.

Oral doses of heavy water in the multi-gram range, along with heavy oxygen ^{18}O, are routinely used in human metabolic experiments. See doubly-labeled water testing. Since 1 in every 6400 hydrogen atoms is deuterium, a 50 kg human containing 32 kg of body water would normally contain enough deuterium (about 1.1 gram) to make 5.5 grams of pure heavy water, so roughly this dose is required to double the amount of deuterium in the body.

6 . Confused report of a " heavy water " contamination incident :

In 1990, a disgruntled employee at the Point Lepreau Nuclear Generating Station in Canada obtained a sample (estimated as about a "half cup") of heavy water from the primary heat transport loop of the nuclear reactor, and loaded it into the employee water cooler. Eight employees drank some of the contaminated water. The incident was discovered when employees began leaving bioassay urine samples with elevated tritium levels. The quantity of heavy water involved was far below levels that could induce heavy water toxicity, but several employees received elevated radiation doses from tritium and neutron-activated chemicals in the water.[10] This was not an incident of heavy water poisoning, but rather radiation poisoning from other isotopes in the heavy water. Some news services were not careful to distinguish these points, and some of the public was left with the impression that heavy water is normally radioactive and more severely toxic than it is. Even if pure heavy water had been used in the water cooler indefinitely, it is not likely the incident would have been detected or caused harm, since no employees would be expected to get as much as 25% of their daily drinking water from such a source.

7 . Production

On Earth, semiheavy water, HDO, occurs naturally in regular water at a proportion of about 1 molecule in 3200. This means that 1 in 6400 hydrogen atoms is deuterium, which is 1 part in 3200 by weight (hydrogen weight). The HDO may be separated from regular water by distillation or electrolysis and also by various chemical exchange processes, all of which exploit a kinetic isotope effect. (For more information about the isotopic distribution of deuterium in water, see Vienna Standard Mean Ocean Water.)

The difference in mass between the two hydrogen isotopes translates into a difference in the zero - point energy and thus into a slight difference in the speed at which the reaction proceeds. Once HDO becomes a significant fraction of the water, heavy water will become more prevalent as water molecules trade hydrogen atoms very frequently. To produce pure heavy water by distillation or electrolysis requires a large cascade of stills or electrolysis chambers, and consumes large amounts of power, so the chemical methods are generally preferred. The most important chemical method is the Girdler sulfide process.

7 . 1 . United States

In 1953, the United States began using heavy water in plutonium production reactors at the Savannah River Site. The first of the five heavy water reactors came online in 1953, and the last was placed in cold shutdown in 1996. The SRS reactors were heavy water reactors so that they could produce both plutonium and tritium for the US nuclear weapons program.

The U.S. developed the Girdler Sulfide chemical exchange production process which was first demonstrated on a large scale at the Dana, Indiana plant in 1945 and at the Savannah River Plant, South Carolina in 1952. The SRP was operated by DuPont for the USDOE until April 1, 1989 at which time the operation was taken over by Westinghouse.

7 . 2 . Norway

In 1934, Norsk Hydro built the first commercial heavy water plant at Vemork, Tinn, with a capacity of 12 tonnes per year. From 1940 and throughout World War II, the plant was under German control and the allies decided to destroy the plant and its heavy water to inhibit German development of nuclear weapons. In late 1942, a planned raid by British airborne troops failed, both gliders crashing.

The raiders were killed in the crash or subsequently executed by the Germans. But in the night of 27 February 1943 Operation Gunnerside succeeded. Norwegian commandos and local resistance managed to demolish small but key parts of the electrolytic cells, dumping the accumulated heavy water down the factory drains. Had the German nuclear program followed similar lines of research as the U.S. Manhattan Project, such heavy water would have been crucial to obtaining plutonium from a nuclear reactor. The Norsk Hydro operation is one of the great commando/sabotage operations of the war.

On 16 November 1943, the allied air forces dropped more than 400 bombs on the site. The allied air raid prompted the Nazi government to move all available heavy water to Germany for safekeeping. On 20 February 1944, a Norwegian partisan sank the ferry M 0/ F *Hydro* carrying the heavy water across Lake Tinn, at the cost of 14 Norwegian civilians, and most of the heavy water was presumably lost. A few of the barrels were only half full, and therefore could float, and may have been salvaged and transported to Germany.

However, recent investigation of production records at Norsk Hydro and analysis of an intact barrel that was salvaged in 2004 revealed that although the barrels in this shipment contained water of pH 14 — indicative of the alkaline electrolytic refinement process - they did not contain high concentrations of D_2O . Despite the apparent size of shipment, the total quantity of pure heavy water was quite small, most barrels only containing between 1 / 2 - 1 % pure heavy water. The Germans would have needed a total of about 5 tons of heavy water to get a nuclear reactor running. The manifest clearly indicated that there was only half a ton of heavy water being transported to Germany. The Hydro was carrying far too little heavy water for even one reactor, let alone the 10 or more tons needed to make enough plutonium for a nuclear weapon. The Hydro shipment on 20 February 1944 was probably destined for an experimental reactor project ·

7 . 3 . Canada

As part of its contribution to the Manhattan Project, Canada built and operated a 6 tonnes per year electrolytic heavy water plant at Trail, BC, which started operation in 1943.

The Atomic Energy of Canada Limited (AECL) design of power reactor requires large quantities of heavy water to act as a neutron moderator and coolant. AECL ordered two heavy water plants which were built and operated in Atlantic Canada at Glace Bay (by Deuterium of Canada Limited) and Port Hawkesbury, Nova Scotia (by General Electric Canada). These plants proved to have significant design, construction and production problems and so AECL built the Bruce Heavy Water Plant, which it later sold to Ontario Hydro, to ensure a reliable supply of heavy water for future power plants. The two Nova Scotia plants were shut down in 1985 when their production proved to be unnecessary.

The Bruce Heavy Water Plant in Ontario was the world's largest heavy water production plant with a capacity of 700 tonnes per year. It used the Girdler sulfide process to produce heavy water, and required 340,000 tonnes of feed water to produce one tonne of heavy water. It was part of a complex that included 8 CANDU reactors which provided heat and power for the heavy water plant. The site was located at Douglas Point in Bruce County on Lake Huron where it had access to the waters of the Great Lakes.

The Bruce plant was commissioned in 1979 to provide heavy water for a large increase in Ontario's nuclear power generation. The plants proved to be significantly more efficient than planned and only three of the planned four units were eventually commissioned. In addition, the nuclear power programme was slowed down and effectively stopped due to a perceived oversupply of electricity, later shown to be temporary, in 1993. Improved efficiency in the use and recycling of heavy water plus the over-production at Bruce left Canada with enough heavy water for its anticipated future needs. Also, the Girdler process involves large amounts of hydrogen sulfide, raising environmental concerns if there should be a release. The Bruce heavy-water plant was shut down in 1997, after which the plant was gradually dismantled and the site cleared.

Atomic Energy of Canada Limited (AECL) is currently researching other more efficient and environmentally benign processes for creating heavy water. This is essential for the future of the CANDU reactors since heavy water represents about 20% of the capital cost of each reactor.

7 . 4 . India

India is the world's second largest producer of heavy water through its Heavy Water Board.

7 . 5 . Iran

On August 26, 2006, Iranian President Ahmadi nejad inaugurated an expansion of the country's heavy-water plant near Arak. Iran has indicated that the heavy - water production facility will operate in tandem with a 40 MW research reactor that has a scheduled completion date in 2009.[13] In an interview which aired on the Iranian News Channel (IRINN) on August 27, 2006, Iranian Nuclear Chief Mohammad Sa'idi claimed that heavy water could be used to treat AIDS and cancer. Daily consumption was recommended.[14]

7 . 6 . Pakistan

The 50 MWt, heavy water and natural uranium research reactor at Khushab, in Punjab province, is a central element of Pakistan's program for production of plutonium, deuterium and tritium for advanced compact warheads.Pakistan succeeded in illicitly acquiring a tritium purification and storage plant, and deuterium and tritium precursor materials from two German firms.Khushab Heavy Water Plant

7 . 7 . Other countries

Argentina is another declared producer of heavy water, using an ammonia / hydrogen exchange based plant supplied by Switzerland's Sulzer company.

Romania also produces heavy water at the Drobeta Girdler Sulfide plant and is exporting it from time to time.

France operated a small plant during the 1950s and 1960s.

8 . Applications

8 . 1 . Nuclear magnetic resonance

Deuterium oxide is used in nuclear magnetic resonance spectroscopy when the solvent of interest is water and the nuclide of interest is hydrogen. This is because the signal from the water solvent would interfere with the signal from the molecule of interest. Deuterium has a different magnetic moment from hydrogen and therefore does not contribute to the NMR signal at the hydrogen resonance frequency.

8 . 2 . Organic Chemistry

Deuterium oxide is often used as the source of deuterium for preparing specifically-labelled isotopologs of organic compounds. For example, C - H bonds adjacent to ketonic carbonyl groups can be replaced by C - D bonds, using acid or base catalysis. Trimethylsulfoxonium iodide, made from dimethylsulfoxide and methyl iodide can be recrystallized from deuterium oxide, and then dissociated to regenerate methyl iodide and dimethylsulfoxide, both deuterium labeled. In cases where specific double labelling by deuterium and tritium is contemplated, the researcher needs to be aware that deuterium oxide, depending upon age and origin, can contain some tritium.

8 . 3 . Fourier Transform Spectroscopy

Deuterium oxide is often used instead of water when collecting FTIR spectra of proteins in solution. H_2O creates a strong band that overlaps with the amide I region of proteins. The band from D_2O is shifted away from the amide I region.

8 . 4 . Neutron moderator

Heavy water is used in certain types of nuclear reactors where it acts as a neutron moderator to slow down neutrons so that they can react with the uranium in the reactor. The CANDU reactor uses this design. Light water also acts as a moderator but because light water absorbs more neutrons than heavy water, reactors using light water must use enriched uranium rather than natural uranium, otherwise criticality is impossible. The use of heavy water essentially increases the efficiency of the nuclear reaction.

Because of this, heavy water reactors will be more efficient at breeding plutonium (from uranium - 238) or uranium - 233 (from thorium - 232) than a comparable light - water reactor, leading them to be of greater concern in regards to nuclear proliferation. The breeding and extraction of plutonium can be a relatively rapid and cheap route to building a nuclear weapon, as chemical separation of plutonium from fuel is easier than isotopic separation of U-235 from natural uranium. Heavy water moderated research reactors or specifically - built plutonium breeder reactors have been used for this purpose by most, if not all, states which possess nuclear weapons, although historically the first nuclear weapons were produced without it. (Pure carbon may be used as a moderator, even in unenriched uranium nuclear reactors. Thus, in the U.S., the first experimental atomic reactor (1942), as well as the Manhattan Project Hanford production reactors which produced the plutonium for the Trinity test and Fat Man bombs, all used pure carbon neutron moderators and functioned with neither enriched uranium nor heavy water).

There is no evidence that civilian heavy water power reactors, such as the CANDU or Atucha designs, have been used for military production of fissile materials. In states which do not already possess nuclear weapons, the nuclear material at these facilities is under IAEA safeguards to discourage any such diversion.

Due to its potential for use in nuclear weapons programs, the possession or import/export of large industrial quantities of heavy water are subject to government control in several countries.

Suppliers of heavy water and heavy water production technology typically apply IAEA (International Atomic Energy Agency) administered safeguards and material accounting to heavy water. (In Australia, the *Nuclear Non-Proliferation (Safeguards) Act 1987*.) In the U.S. and Canada, non-industrial quantities of heavy water (i.e., in the gram to kg range) are routinely available through chemical supply dealers, and directly commercial companies such as the world's former major producer Ontario Hydro, without special license. Current (2006) cost of a kilogram of 99.98 % reactor - purity heavy water, is about $ 600 to $700. Smaller quantities of reasonable purity (99.9 %) may be purchased from chemical supply houses at prices of roughly $1 per gram.

8 . 5 . Neutrino detector

The Sudbury Neutrino Observatory (SNO) in Sudbury, Ontario used 1000 tonnes of heavy water on loan from Atomic Energy of Canada Limited. The neutrino detector is 6800 feet underground in a deep mine, in order to shield it from muons produced by cosmic rays. SNO was built to answer the question of whether or not electron-type neutrinos produced by fusion in the Sun (the only type the Sun should be producing directly, according to theory) might be able to turn into other types of neutrinos on the way to Earth. SNO detects the Čerenkov radiation in the water from high - energy electrons produced from electron-type neutrinos as they undergo reactions with neutrons in deuterium, turning them into protons and electrons (only the electrons move fast enough to be detected in this manner). SNO also detects the same radiation from neutrino ↔ electron scattering events, which again produces high energy electrons. These two reactions are produced only by electron - type neutrinos. The use of deuterium is critical to the SNO function, because all three "flavours" (types) of neutrinos[15] may be detected in a third type of reaction, neutrino-disintegration, in which a neutrino of any type (electron, muon, or tau) scatters from a deuterium nucleus (deuteron), transferring enough energy to break up the loosely-bound deuteron into a free neutron and proton. This event is detected when the free neutron is absorbed by $^{35}Cl^{-}$ present from NaCl which has been deliberately dissolved in the heavy water, causing emission of characteristic capture gamma rays. Thus, in this experiment, heavy water not only provides the transparent medium necessary to produce and visualize Čerenkov radiation, but it also provides deuterium to detect exotic mu type (μ) and tau (τ) neutrinos, as well as a non-absorbent moderator medium to preserve free neutrons from this reaction, until they can be absorbed by an easily - detected neutron-activated isotope.

8 . 6 . Metabolic rate testing in physiology/biology

Heavy water is employed as part of a mixture with $H_2{}^{18}O$ for a common and safe test of mean metabolic rate in humans and animals undergoing their normal activities. This metabolic test is usually called the doubly-labeled water test.

8 . 7 . Tritium production

Tritium is an important material in nuclear weapon design for boosted fission weapons and initiators, and also has civilian industrial applications. Some is created in heavy water moderated reactors when deuterium captures a neutron. This reaction has a small cross-section and produces only small amounts of tritium, although enough so that cleaning tritium from the moderator may be desirable after several years to reduce the risk of tritium escape and radiation exposure.

Production of large amounts of tritium in this way would require reactors with very high neutron fluxes, or with a very high proportion of heavy water to nuclear fuel and very low neutron absorption by other reactor material. The tritium would then have to be recovered by isotope separation from a much larger quantity of deuterium, unlike tritium production from lithium - 6 (the present method of tritium production), where only chemical separation is needed . Deuterium's absorption cross section for thermal neutrons is .52 millibarns, while oxygen-16's is .19 millibarns and oxygen-17's is .24 barn. ^{17}O makes up .038 % of natural oxygen, which has an overall absorption cross section of .28 millibarns. Therefore in D_2O with natural oxygen, 21 % of neutron captures are on oxygen, a proportion that may rise further as ^{17}O accumulates from neutron capture on ^{16}O. Also, ^{17}O emits an alpha particle on capture, producing radioactive carbon - 14.

Water

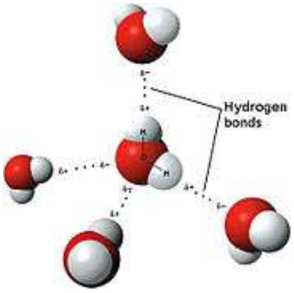
Contents

1 . Introduction :

Water is a ubiquitous chemical substance, composed of hydrogen and oxygen, that is essential for the survival of all known forms of life . In typical usage, *water* refers only to its liquid form or state, but the substance also has a solid state, ice, and a gaseous state, water vapor or steam. Water covers 71 % of the Earth's surface . On Earth, it is found mostly in oceans and other large water bodies, with 1.6% of water below ground in aquifers and 0.001 % in the air as vapor, clouds (formed of solid and liquid water particles suspended in air), and precipitation. Saltwater oceans hold 97 % of surface water, glaciers and polar ice caps 2.4 %, and other land surface water such as rivers, lakes and ponds 0.6 %. A very small amount of the Earth's water is contained within biological bodies and manufactured products. Other water is trapped in ice caps, glaciers, aquifers, or in lakes, sometimes providing fresh water for life on land.Water moves continually through a cycle of evaporation or transpiration (evapotranspiration), precipitation, and runoff, usually reaching the sea. Winds carry water vapor over land at the same rate as runoff into the sea. Over land, evaporation and transpiration contribute to the precipitation over land.

Clean, fresh drinking water is essential to human and other lifeforms. Access to safe drinking water has improved steadily and substantially over the last decades in almost every part of the world.[3][4] There is a clear correlation between access to safe water and GDP per capita. However, some observers have estimated that by 2025 more than half of the world population will be facing water-based vulnerability . Water plays an important role in the world economy, as it functions as a solvent for a wide variety of chemical substances and facilitates industrial cooling and transportation. Approximately 70 percent of freshwater is consumed by agriculture.

2 . Chemical and physical properties



Model of hydrogen bonds between molecules of water

Impact from a water drop causes an upward "rebound" jet surrounded by circular capillary waves.

Capillary action of water compared to mercury . Water is the chemical substance with chemical formula **H_2O** : one molecule of water has two hydrogen atoms covalently bonded to a single oxygen atom.

Water appears in nature in all three common states of matter and may take many different forms on Earth: water vapor and clouds in the sky; seawater and icebergs in the polar oceans; glaciers and rivers in the mountains; and the liquid in aquifers in the ground.

The major chemical and physical properties of water are:

- Water is a tasteless, odorless liquid at standard temperature and pressure. The color of water and ice is, intrinsically, a very light blue hue, although water appears colorless in small quantities. Ice also appears colorless, and water vapor is essentially invisible as a gas.

- Water is transparent, and thus aquatic plants can live within the water because sunlight can reach them. Only strong UV light is slightly absorbed.

- Since oxygen has a higher electronegativity than hydrogen, water is a polar molecule. The oxygen has a slight negative charge while the hydrogens have a slight positive charge giving the article a strong effective dipole moment. The interactions between the different dipoles of each molecule cause a net attraction force associated with water's high amount of surface tension.

- The dipolar nature contributes to water molecules' tendency to form hydrogen bonds which cause water's cohesive properties.

- Water has a high surface tension caused by the weak interactions, (Van Der Waals Force) between water molecules because it is polar. The apparent elasticity caused by surface tension drives the capillary waves.

- Water also has high adhesion properties because of its polar nature.

- Capillary action refers to the tendency of water to move up a narrow tube against the force of gravity. This property is relied upon by all vascular plants, such as trees.

- Water is a very strong solvent and is often referred to as *the universal solvent*. Substances that dissolve in water, e.g. salts, sugars, acids, alkalis, and some gases – especially oxygen, carbon dioxide (carbonation) – are known as "hydrophilic" (water - loving) substances, while those that do not mix well with water (e.g. fats and oils), are known as " hydrophobic " (water - fearing) substances.

- All the major components in cells (proteins, DNA and polysaccharides) are also dissolved in water.

- Pure water has a *low* electrical conductivity, but this increases significantly with the dissolution of a small amount of ionic material such as sodium chloride.

- The boiling point of water (and all other liquids) is related to the barometric pressure. For example, on the top of Mt. Everest water boils at about 68 °C (154 °F), compared to 100 °C (212 °F) at sea level. Conversely, water deep in the ocean near geothermal vents can reach temperatures of hundreds of degrees and remain liquid.

- Water has the second highest specific heat capacity of any known substance, after ammonia, as well as a high heat of vaporization (40.65 $\text{kJ}\cdot\text{mol}^{-1}$) , both of which are a result of the extensive hydrogen bonding between its molecules. These two unusual properties allow water to moderate Earth's climate by buffering large fluctuations in temperature.

- The maximum density of water occurs at 3.98 °C. Water becomes even less dense upon freezing, expanding 9 %. This results in an unusual phenomenon: water's solid form, ice, floats upon water, allowing organisms to survive inside a partially-frozen water body because the water on the bottom has a temperature of around 4 °C .

ADR label for transporting goods dangerously reactive with water

- Water is miscible with many liquids, for example ethanol, in all proportions, forming a single homogeneous liquid. On the other hand, water and most oils are *immiscible* usually forming layers according to increasing density from the top. As a gas, water vapor is completely miscible with air.

- Water forms an azeotrope with many other solvents.

- Water can be split by electrolysis into hydrogen and oxygen.

- As an oxide of hydrogen, water is formed when hydrogen or hydrogen-containing compounds burn or react with oxygen or oxygen-containing compounds. Water is not a fuel, it is an end-product of the combustion of hydrogen. The energy required to split water into hydrogen and oxygen by electrolysis or any other means is greater than the energy released when the hydrogen and oxygen recombine.

- Elements which are more electropositive than hydrogen such as lithium, sodium, calcium, potassium and caesium displace hydrogen from water, forming hydroxides. Being a flammable gas, the hydrogen given off is dangerous and the reaction of water with the more electropositive of these elements may be violently explosive.

- At ultrahigh pressures found in deep interiors of giant planets Uranus and Neptune water may become metallic, which would have important implications for the generation of the magnetic fields of these planets.

3 . Taste and odor

Water can dissolve many different substances, giving it varying tastes and odors. In fact, humans and other animals have developed senses which are, to a degree, able to evaluate the potability of water, avoiding water that is too salty or putrid. Humans also tend to prefer cold water to lukewarm water; cold water is likely to contain fewer microbes. The taste advertised in spring water or mineral water derives from the minerals dissolved in it, as pure H_2O is tasteless and odorless. As such, purity in spring and mineral water refers to absence of toxins, pollutants, and microbes.

4 . Distribution of water in nature

4 . 1 . Water in the universe

Much of the universe's water may be produced as a byproduct of star formation. When stars are born, their birth is accompanied by a strong outward wind of gas and dust. When this outflow of material eventually impacts the surrounding gas, the shock waves that are created compress and heat the gas. The water observed is quickly produced in this warm dense gas.

Water has been detected in interstellar clouds within our galaxy, the Milky Way. It is believed that water exists in abundance in other galaxies too, because its components, hydrogen and oxygen, are among the most abundant elements in the universe. Interstellar clouds eventually condense into solar nebulae and solar systems, such as ours.

Water vapor is present on :

- Mercury - 3.4 % in the atmosphere, and large amounts of water in Mercury's exosphere .
- Venus - 0.002 % in the atmosphere
- Earth - trace in the atmosphere (varies with climate)

- Mars - 0.03 % in the atmosphere
- Jupiter - 0.0004 % in the atmosphere
- Saturn - in ices only
- Enceladus (moon of Saturn) – 91 % in the atmosphere
- exoplanets known as HD 189733 b and HD 209458 b .

Liquid water is present on :

- Earth – 71 % of surface
- Moon - small amounts of water have been found (in 2008) in the inside of volcanic pearls brought from Moon to Earth by the Apollo 15 crew in 1971.

Strong evidence suggests that liquid water is present just under the surface of Saturn's moon Enceladus and on Jupiter's moon Europa.

Water ice is present on :

- Earth - mainly on ice sheets
- polar ice caps on Mars
- Titan
- Europa
- Enceladus
- Comets and comet source populations (Kuiper belt and Oort cloud objects).

Water ice may be contained on the Moon, Ceres and Tethys. Water and other volatiles probably comprise much of the internal structures of Uranus and Neptune.

4 . 2 . Water and habitable zone

The Solar System along center row range of possible habitable zones of varying size stars.

The existence of liquid water, and to a lesser extent its gaseous and solid forms, on Earth is vital to the existence of life on Earth as we know it. The Earth is located in the habitable zone of the solar system; if it were slightly closer to or further from the Sun (about 5 %, or about 8 million kilometres), the conditions which allow the three forms to be present simultaneously would be far less likely to exist .

Earth's gravity allows it to hold an atmosphere. Water vapor and carbon dioxide in the atmosphere provide a temperature buffer (greenhouse effect) which helps maintain a relatively steady surface temperature. If Earth were smaller, a thinner atmosphere would allow temperature extremes, thus preventing the accumulation of water except in polar ice caps (as on Mars).

It has been proposed that life itself may maintain the conditions that have allowed its continued existence . The surface temperature of Earth has been relatively constant through geologic time despite varying levels of incoming solar radiation (insolation), indicating that a dynamic process governs Earth's temperature via a combination of greenhouse gases and surface or atmospheric albedo. This proposal is known as the *Gaia hypothesis*.

The state of water on a planet depends on ambient pressure, which is determined by the planet's gravity. If a planet is sufficiently massive, the water on it may be solid even at high temperatures, because of the high pressure caused by gravity.

There are various theories about origin of water on Earth.

5 . Hydrology and Water distribution on Earth

Water covers 71 % of the Earth's surface; the oceans contain 97.2 % of the Earth's water. The Antarctic ice sheet, which contains 90 % of all fresh water on Earth, is visible at the bottom. Condensed atmospheric water can be seen as clouds, contributing to the Earth's albedo.

Hydrology is the study of the movement, distribution, and quality of water throughout the Earth. The study of the distribution of water is hydrography. The study of the distribution and movement of groundwater is hydrogeology, of glaciers is glaciology, of inland waters is limnology and distribution of oceans is oceanography. Ecological processes with hydrology are in focus of ecohydrology.

The collective mass of water found on, under, and over the surface of a planet is called the hydrosphere. Earth's approximate water volume (the total water supply of the world) is 1,360,000,000 km^3 .

A graphical distribution of the locations of water on Earth :

- 1,320,000,000 km^3 (or 97.2%) is in the oceans.
- 25,000,000 km^3 (or 1.8 %) is in glaciers, ice caps and ice sheets.
- 13,000,000 km^3 (or 0.9 %) is groundwater.
- 250,000 km^3 (or 0.02 %) is fresh water in lakes, inland seas, and rivers.
- 13,000 km^3 (or 0.001 %) is atmospheric water vapor at any given time.

Ground water and fresh water are useful or potentially useful to humans as water resources.

Liquid water is found in bodies of water, such as an ocean, sea, lake, river, stream, canal, pond, or puddle. The majority of water on Earth is sea water. Water is also present in the atmosphere in solid, liquid, and vapor states. It also exists as groundwater in aquifers.

Water is important in many geological processes. Groundwater is ubiquitous in rocks, and the pressure of this groundwater affects patterns of faulting. Water in the mantle is responsible for the melt that produces volcanoes. On the surface of the Earth, water is important in both chemical and physical weathering processes. Water and, to a lesser but still significant extent, ice, are also responsible for a large amount of sediment transport that occurs on the surface of the earth. Deposition of transported sediment forms many types of sedimentary rocks, which make up the geologic record of Earth history.

5 . 1 . Water cycle

The water cycle (known scientifically as the **hydrologic cycle**) refers to the continuous exchange of water within the hydrosphere, between the atmosphere, soil water, surface water, groundwater, and plants.

Water moves perpetually through each of these regions in the *water cycle* consisting of following transfer processes:

- evaporation from oceans and other water bodies into the air and transpiration from land plants and animals into air.
- precipitation, from water vapor condensing from the air and falling to earth or ocean.
- runoff from the land usually reaching the sea.

Most water vapor over the oceans returns to the oceans, but winds carry water vapor over land at the same rate as runoff into the sea, about 36 Tt per year. Over land, evaporation and transpiration contribute another 71 Tt per year. Precipitation, at a rate of 107 Tt per year over land, has several forms: most commonly rain, snow, and hail, with some contribution from fog and dew. Condensed water in the air may also refract sunlight to produce rainbows.

Water runoff often collects over watersheds flowing into rivers. A mathematical model used to simulate river or stream flow and calculate water quality parameters is hydrological transport model. Some of water is diverted to irrigation for agriculture. Rivers and seas offer opportunity for travel and commerce. Through erosion, runoff shapes the environment creating river valleys and deltas which provide rich soil and level ground for the establishment of population centers. A flood occurs when an area of land, usually low - lying, is covered with water. It is when a river overflows its banks or flood from the sea. A drought is an extended period of months or years when a region notes a deficiency in its water supply. This occurs when a region receives consistently below average precipitation.

5 . 2 . Fresh water resources

Some runoff water is trapped for periods, for example in lakes. At high altitude, during winter, and in the far north and south, snow collects in ice caps, snow pack and glaciers. Water also infiltrates the ground and goes into aquifers. This groundwater later flows back to the surface in springs, or more spectacularly in hot springs and geysers. Groundwater is also extracted artificially in wells. This water storage is important, since clean, fresh water is essential to human and other land - based life. In many parts of the world, it is in short supply.

5 . 3 . Tides

Tides are the cyclic rising and falling of Earth's ocean surface caused by the tidal forces of the Moon and the Sun acting on the oceans. Tides cause changes in the depth of the marine and estuarine water bodies and produce oscillating currents known as tidal streams. The changing tide produced at a given location is the result of the changing positions of the Moon and Sun relative to the Earth coupled with the effects of Earth rotation and the local bathymetry. The strip of seashore that is submerged at high tide and exposed at low tide, the intertidal zone, is an important ecological product of ocean tides.

6 . Effects on life

From a biological standpoint, water has many distinct properties that are critical for the proliferation of life that set it apart from other substances. It carries out this role by allowing organic compounds to react in ways that ultimately allow replication. All known forms of life depend on water. Water is vital both as a solvent in which many of the body's solutes dissolve and as an essential part of many metabolic processes within the body. Metabolism is the sum total of anabolism and catabolism. In anabolism, water is removed from molecules (through energy requiring enzymatic chemical reactions) in order to grow larger molecules (e.g. starches, triglycerides and proteins for storage of fuels and information). In catabolism, water is used to break bonds in order to generate smaller molecules (e.g. glucose, fatty acids and amino acids to be used for fuels for energy use or other purposes). Water is thus essential and central to these metabolic processes. Therefore, without water, these metabolic processes would cease to exist, leaving us to muse about what processes would be in its place, such as gas absorption, dust collection, etc.

Overview of photosynthesis and respiration. Water (at right), together with carbon dioxide (CO_2), form oxygen and organic compounds (at left), which can be respired to water and (CO_2).

Water is also central to photosynthesis and respiration. Photosynthetic cells use the sun's energy to split off water's hydrogen from oxygen. Hydrogen is combined with CO_2 (absorbed from air or water) to form glucose and release oxygen. All living cells use such fuels and oxidize the hydrogen and carbon to capture the sun's energy and reform water and CO_2 in the process (cellular respiration).

Water is also central to acid-base neutrality and enzyme function. An acid, a hydrogen ion (H^+, that is, a proton) donor, can be neutralized by a base, a proton acceptor such as hydroxide ion (OH^-) to form water. Water is considered to be neutral, with a pH (the negative log of the hydrogen ion concentration) of 7. Acids have pH values less than 7 while bases have values greater than 7. Stomach acid (HCl) is useful to digestion. However, its corrosive effect on the esophagus during reflux can temporarily be neutralized by ingestion of a base such as aluminum hydroxide to produce the neutral molecules water and the salt aluminum chloride. Human biochemistry that involves enzymes usually performs optimally around a biologically neutral pH of 7.4.

For example a cell of *Escherichia coli* contains 70 % of water, a human body 60 – 70 %, plant body up to 90% and the body of an adult jellyfish is made up of 94 – 98 % water.

6 . 1 . Aquatic life forms :

Earth's waters are filled with life. The earliest life forms appeared in water; nearly all fish live exclusively in water, and there are many types of marine mammals, such as dolphins and whales that also live in the water. Some kinds of animals, such as amphibians, spend portions of their lives in water and portions on land. Plants such as kelp and algae grow in the water and are the basis for some underwater ecosystems. Plankton is generally the foundation of the ocean food chain.

Aquatic animals must obtain oxygen to survive, and they do so in various ways. Fish have gills instead of lungs, although some species of fish, such as the lungfish, have both. Marine mammals, such as dolphins, whales, otters, and seals need to surface periodically to breathe air. Smaller life forms are able to absorb oxygen through their skin.

7 . Effects on human civilization

Civilization has historically flourished around rivers and major waterways; Mesopotamia, the so-called cradle of civilization, was situated between the major rivers Tigris and Euphrates; the ancient society of the Egyptians depended entirely upon the Nile. Large metropolises like Rotterdam, London, Montreal, Paris, New York City, Buenos Aires, Shanghai, Tokyo, Chicago, and Hong Kong owe their success in part to their easy accessibility via water and the resultant expansion of trade. Islands with safe water ports, like Singapore, have flourished for the same reason. In places such as North Africa and the Middle East, where water is more scarce, access to clean drinking water was and is a major factor in human development.

7 . 1 . Health and pollution

Water fit for human consumption is called drinking water or potable water. Water that is not potable can be made potable by filtration or distillation (heating it until it becomes water vapor, and then capturing the vapor without any of the impurities it leaves behind), or by other methods (chemical or heat treatment that kills bacteria). Sometimes the term safe water is applied to potable water of a lower quality threshold (i.e., it is used effectively for nutrition in humans that have weak access to water cleaning processes, and does more good than harm). Water that is not fit for drinking but is not harmful for humans when used for swimming or bathing is called by various names other than potable or drinking water, and is sometimes called safe water, or "safe for bathing". Chlorine is a skin and mucous membrane irritant that is used to make water safe for bathing or drinking. Its use is highly technical and is usually monitored by government regulations (typically 1 part per million (ppm) for drinking water, and 1–2 ppm of chlorine not yet reacted with impurities for bathing water).

This natural resource is becoming scarcer in certain places, and its availability is a major social and economic concern. Currently, about a billion people around the world routinely drink unhealthy water. Most countries accepted the goal of halving by 2015 the number of people worldwide who do not have access to safe water and sanitation during the 2003 G8 Evian summit . Even if this difficult goal is met, it will still leave more than an estimated half a billion people without access to safe drinking water and over a billion without access to adequate sanitation. Poor water quality and bad sanitation are deadly; some five million deaths a year are caused by polluted drinking water. The World Health Organization estimates that safe water could prevent 1.4 million child deaths from diarrhea each year.[20] Water, however, is not a finite resource, but rather re - circulated as potable water in precipitation in quantities many degrees of magnitude higher than human consumption. Therefore, it is the relatively small quantity of water in reserve in the earth (about 1 percent of our drinking water supply, which is replenished in aquifers around every 1 to 10 years), that is a non-renewable resource, and it is, rather, the distribution of potable and irrigation water which is scarce, rather than the actual amount of it that exists on the earth. Water - poor countries use importation of goods as the primary method of importing water (to leave enough for local human consumption), since the manufacturing process uses around 10 to 100 times products' masses in water.

In the developing world, 90 % of all wastewater still goes untreated into local rivers and streams . Some 50 countries, with roughly a third of the world’s population, also suffer from medium or high water stress, and 17 of these extract more water annually than is recharged through their natural water cycles . The strain not only affects surface freshwater bodies like rivers and lakes, but it also degrades groundwater resources.

7 . 2 . Human uses

7 . 2 . 1 . Agriculture

The most important use of water in agriculture is for an irrigation and irrigation is key component to produce enough food. Irrigation takes up to 90% of water withdrawn in some developing countries .

7 . 2 . 2 . Water as a scientific standard

On 7 April 1795, the gram was defined in France to be equal to "the absolute weight of a volume of pure water equal to a cube of one hundredth of a metre, and to the temperature of the melting ice."[24] For practical purposes though, a metallic reference standard was required, one thousand times more massive, the kilogram. Work was therefore commissioned to determine precisely the mass of one liter of water. In spite of the fact that the decreed definition of the gram specified water at 0 °C - a highly reproducible *temperature*—the scientists chose to redefine the standard and to perform their measurements at the temperature of highest water *density*, which was measured at the time as 4 °C .

The Kelvin temperature scale of the SI system is based on the triple point of water, defined as exactly 273.16 K or 0.01 °C. The scale is a more accurate development of the Celsius temperature scale, which was originally defined according the boiling point (set to 100 °C) and melting point (set to 0 °C) of water.

Natural water consists mainly of the isotopes hydrogen-1 and oxygen-16, but there is also small quantity of heavier isotopes such as hydrogen - 2 (deuterium). The amount of deuterium oxides or heavy water is very small, but it still affects the properties of water. Water from rivers and lakes tends to contain less deuterium than seawater. Therefore, standard water is defined in the Vienna Standard Mean Ocean Water specification.

7 . 2 . 3 . For drinking

The human body is anywhere from 55 % to 78 % water depending on body size.[26] To function properly, the body requires between one and seven liters of water per day to avoid dehydration; the precise amount depends on the level of activity, temperature, humidity, and other factors. Most of this is ingested through foods or beverages other than drinking straight water. It is not clear how much water intake is needed by healthy people, though most advocates agree that 6 – 7 glasses of water (approximately 2 litres) daily is the minimum to maintain proper hydration . Medical literature favors a lower consumption, typically 1 liter of water for an average male, excluding extra requirements due to fluid loss from exercise or warm weather.[28] For those who have healthy kidneys, it is rather difficult to drink too much water, but (especially in warm humid weather and while exercising) it is dangerous to drink too little. People can drink far more water than necessary while exercising, however, putting them at risk of water intoxication (hyperhydration), which can be fatal. The "fact" that a person should consume eight glasses of water per day cannot be traced back to a scientific source.[29] There are other myths such as the effect of water on weight loss and constipation that have been dispelled .

An original recommendation for water intake in 1945 by the Food and Nutrition Board of the National Research Council read: " An ordinary standard for diverse persons is 1 milliliter for each calorie of food. Most of this quantity is contained in prepared foods."[31] The latest dietary reference intake report by the United States National Research Council in general recommended (including food sources) : 2.7 liters of water total for women and 3.7 liters for men.[32] Specifically, pregnant and breastfeeding women need additional fluids to stay hydrated. According to the Institute of Medicine—who recommend that, on average, women consume 2.2 litres and men 3.0 litres—this is recommended to be 2.4 litres (10 cups) for pregnant women and 3 litres (12 cups) for breastfeeding women since an especially large amount of fluid is lost during nursing . Also noted is that normally, about 20 percent of water intake comes from food, while the rest comes from drinking water and beverages (

caffeinated included). Water is excreted from the body in multiple forms; through urine and feces, through sweating, and by exhalation of water vapor in the breath. With physical exertion and heat exposure, water loss will increase and daily fluid needs may increase as well.

Hazard symbol for *No drinking water* :

Humans require water that does not contain too many impurities. Common impurities include metal salts and oxides (including copper, iron, calcium and lead) and/or harmful bacteria, such as *Vibrio*. Some solutes are acceptable and even desirable for taste enhancement and to provide needed electrolytes.

The single largest freshwater resource suitable for drinking is Lake Baikal in Siberia, which has a very low salt and calcium content and is therefore very clean.

7 . 2 . 4 . As a dissolving agent or solvent

Dissolving (or suspending) is used to wash everyday items such as the human body, clothes, floors, cars, food, and pets. Also, human wastes are carried by water in the sewage system. Its use as a cleaning solvent consumes most of water in industrialized countries.

Water can facilitate the chemical processing of wastewater. An aqueous environment can be favorable to the breakdown of pollutants, due to the ability to gain a homogeneous solution that can be pumped and is easier to treat. Aerobic treatment can be used by applying oxygen or air to a solution reduce the reactivity of substances within it.

Water also facilitates biological processing of waste that have been dissolved within it. Microorganisms that live within water can access dissolved wastes and can feed upon them breaking them down into less polluting substances. Reedbeds and anaerobic digesters are both examples of biological systems that are particularly suited to the treatment of effluents.

Typically from both chemical and biological treatment of wastes, there is often a solid residue or cake that is left over from the treatment process. Depending upon its constituent parts, this 'cake' may be dried and spread on land as a fertilizer if it has beneficial properties, or alternatively disposed of in landfill or incinerated.

7 . 2 . 5 . As a heat transfer fluid

Water and steam are used as heat transfer fluids in diverse heat exchange systems, due to its availability and high heat capacity, both as a coolant and for heating. Cool water may even be naturally available from a lake or the sea. Condensing steam is a particularly efficient heating fluid because of the large heat of vaporization. A disadvantage is that water and steam are somewhat corrosive. In almost all electric power plants, water is the coolant, which vaporizes and drives steam turbines to drive generators.

In the nuclear industry, water can also be used as a neutron moderator. In a pressurized water reactor, water is both a coolant and a moderator. This provides a passive safety measure, as removing the water from the reactor also slows the nuclear reaction down.

7 . 2 . 6 . Extinguishing fires

Water has a high heat of vaporization and is relatively inert, which makes it a good fire extinguishing fluid. The evaporation of water carries heat away from the fire. However, water cannot be used to fight fires of electric equipment, because impure water is electrically conductive, or of oils and organic solvents, because they float on water and the explosive boiling of water tends to spread the burning liquid.

Use of water in fire fighting should also take into account the hazards of a steam explosion, which may occur when water is used on very hot fires in confined spaces, and of a hydrogen explosion, when substances which react with water, such as certain metals or hot graphite, decompose the water, producing hydrogen gas.

The power of such explosions was seen in the Chernobyl disaster, although the water involved did not come from fire-fighting at that time but the reactor's own water cooling system. A steam explosion occurred when the extreme over-heating of the core caused water to flash into steam. A hydrogen explosion may have occurred as a result of reaction between steam and hot zirconium.

7 . 2 . 7 . Chemical uses

Organic reactions are usually quenched with water or a water solution of a suitable acid, base or buffer. Water is generally effective in removing inorganic salts. In inorganic reactions, water is a common solvent. In organic reactions, it is usually not used as a reaction solvent, because it does not dissolve the reactants well and is amphoteric (acidic *and* basic) and nucleophilic. Nevertheless, these properties are sometimes desirable. Also, acceleration of Diels-Alder reactions by water has been observed. Supercritical water has recently been a topic of research. Oxygen - saturated supercritical water combusts organic pollutants efficiently.

7 . 2 . 8 . Recreation

Humans use water for many recreational purposes, as well as for exercising and for sports. Some of these include swimming, waterskiing, boating, surfing and diving. In addition, some sports, like ice hockey and ice skating, are played on ice. Lakesides, beaches and waterparks are popular places for people to go to relax and enjoy recreation. Many find the sound of flowing water to be calming, too. Some keep fish and other life in aquariums or ponds for show, fun, and companionship. Humans also use water for snow sports i.e. skiing or snowboarding, which requires the water to be frozen. People may also use water for play fighting such as with snowballs, water guns or water balloons. They may also make fountains and use water in their public or private decorations.

7 . 2 . 9 . Water industry

A water - carrier in India, 1882. In many places where running water is not available, water has to be transported by people.

Main articles: Water industry and :Category:Water supply and sanitation by country

The water industry provides drinking water and wastewater services (including sewage treatment) to households and industry.

Water supply facilities includes for example water wells cisterns for rainwater harvesting, water supply network, water purification facilities, water tanks, water towers, water pipes including old aqueducts. Atmospheric water generator is in development.

Drinking water is often collected at springs, extracted from artificial borings in the ground, or wells. Building more wells in adequate places is thus a possible way to produce more water, assuming the aquifers can supply an adequate flow. Other water sources are rainwater and river or lake water. This surface water, however, must be purified for human consumption. This may involve removal of undissolved substances, dissolved substances and harmful microbes. Popular methods are filtering with sand which only removes undissolved material, while chlorination and boiling kill harmful microbes. Distillation does all three functions. More advanced techniques exist, such as reverse osmosis. Desalination of abundant ocean or seawater is a more expensive solution used in coastal arid climates.

The distribution of drinking water is done through municipal water systems or as bottled water. Governments in many countries have programs to distribute water to the needy at no charge. Others argue that the market mechanism and free enterprise are best to manage this rare resource and to finance the boring of wells or the construction of dams and reservoirs.

Reducing waste by using drinking water only for human consumption is another option. In some cities such as Hong Kong, sea water is extensively used for flushing toilets citywide in order to conserve fresh water resources.

Polluting water may be the biggest single misuse of water; to the extent that a pollutant limits other uses of the water, it becomes a waste of the resource, regardless of benefits to the polluter. Like other types of pollution, this does not enter standard accounting of market costs, being conceived as externalities for which the market cannot account. Thus other people pay the price of water pollution, while the private firms' profits are not redistributed to the local population victim of this pollution. Pharmaceuticals consumed by humans often end up in the waterways and can have detrimental effects on aquatic life if they bioaccumulate and if they are not biodegradable.

Wastewater facilities are storm sewers and wastewater treatment plants. Another way to remove pollution from surface runoff water is bioswale.

7 . 2 . 10 . Industrial applications

Water is used in power generation. Hydroelectricity is electricity obtained from hydropower. Hydroelectric power comes from water driving a water turbine connected to a generator. Hydroelectricity is a low-cost, non-polluting, renewable energy source. The energy is supplied by the sun. Heat from the sun evaporates water, which condenses as rain in higher altitudes, from where it flows down.

Pressurized water is used in water blasting and water jet cutters. Also, very high pressure water guns are used for precise cutting. It works very well, is relatively safe, and is not harmful to the environment. It is also used in the cooling of machinery to prevent over-heating, or prevent saw blades from over-heating.

Water is also used in many industrial processes and machines, such as the steam turbine and heat exchanger, in addition to its use as a chemical solvent. Discharge of untreated water from industrial uses is pollution. Pollution includes discharged solutes (chemical pollution) and discharged coolant water (thermal pollution). Industry requires pure water for many applications and utilizes a variety of purification techniques both in water supply and discharge.

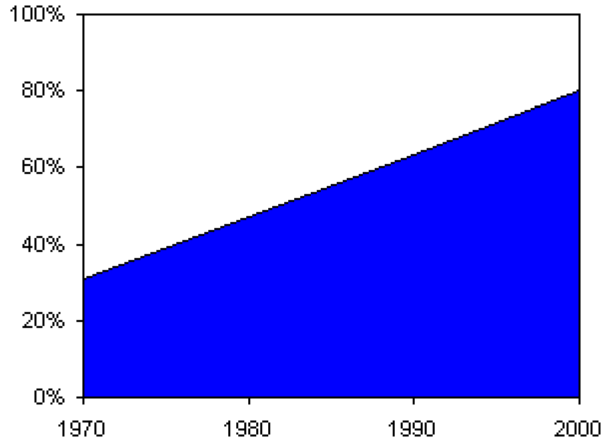
7 . 2 . 11 . Food processing

Water plays many critical roles within the field of food science. It is important for a food scientist to understand the roles that water plays within food processing to ensure the success of their products.

Solutes such as salts and sugars found in water affect the physical properties of water. The boiling and freezing points of water is affected by solutes. One mole of sucrose (sugar) per kilogram of water raises the boiling point of water by 0.51 °C, and one mole of salt per kg raises the boiling point by 1.02 °C; similarly, increasing the number of dissolved particles lowers water's freezing point.[36] Solutes in water also affect water activity which affects many chemical reactions and the growth of microbes in food. Water activity can be described as a ratio of the vapor pressure of water in a solution to the vapor pressure of pure water. Solutes in water lower water activity. This is important to know because most bacterial growth ceases at low levels of water activity. Not only does microbial growth affect the safety of food but also the preservation and shelf life of food . Water hardness is also a critical factor in food processing. It can dramatically affect the quality of a product as well as playing a role in sanitation. Water hardness is classified based on the amounts of removable calcium carbonate salt it contains per gallon. Water hardness is measured in grains; 0.064 g calcium carbonate is equivalent to one grain of hardness. Water is classified as soft if it contains 1 to 4 grains, medium if it contains 5 to 10 grains and hard if it contains 11 to 20 grains . The hardness of water may be altered or treated by using a chemical ion exchange system. The hardness of water also affects its pH balance which plays a critical role in food processing. For example, hard water prevents successful production of clear beverages. Water hardness also affects sanitation; with increasing hardness, there is a loss of effectiveness for its use as a sanitizer.

Boiling, steaming, and simmering are popular cooking methods that often require immersing food in water or its gaseous state, steam. While cooking water is used for dishwashing too.

8 . Water politics and water crisis :



Best estimate of the share of people in developing countries with access to drinking water 1970 – 2000.

Water politics is politics affected by water and water resources. For this reason, water is a strategic resource in the globe and an important element in many political conflicts. It causes health impacts and damage to biodiversity.

1.6 billion people have gained access to a safe water source since 1990. The proportion of people in developing countries with access to safe water is calculated to have improved from 30 percent in 1970[3] to 71 percent in 1990, 79 percent in 2000 and 84 percent in 2004. This trend is projected to continue. To halve, by 2015, the proportion of people without sustainable access to safe drinking water is one of the Millennium Development Goals. This goal is projected to be reached.

A 2006 United Nations report stated that "there is enough water for everyone", but that access to it is hampered by mismanagement and corruption.

UNESCO's World Water Development Report (WWDR, 2003) from its World Water Assessment Program indicates that, in the next 20 years, the quantity of water available to everyone is predicted to decrease by 30 percent. 40 percent of the world's inhabitants currently have insufficient fresh water for minimal hygiene. More than 2.2

million people died in 2000 from waterborne diseases (related to the consumption of contaminated water) or drought. In 2004, the UK charity WaterAid reported that a child dies every 15 seconds from easily preventable water-related diseases; often this means lack of sewage disposal; see toilet.

Organizations concerned in water protection include International Water Association (IWA), WaterAid, Water 1st, American Water Resources Association. Water related conventions are United Nations Convention to Combat Desertification (UNCCD), International Convention for the Prevention of Pollution from Ships, United Nations Convention on the Law of the Sea and Ramsar Convention. World Day for Water takes place on 22 March and World Ocean Day on 8 June . Water used in the production of a good or service is virtual water.

9 . Religion, philosophy, and literature

Water is considered a purifier in most religions. Major faiths that incorporate ritual washing (ablution) include Christianity, Hinduism, Rastafarianism, Islam, Shinto, Taoism, and Judaism. Immersion (or aspersion or affusion) of a person in water is a central sacrament of Christianity (where it is called baptism); it is also a part of the practice of other religions, including Judaism (*mikvah*) and Sikhism (*Amrit Sanskar*). In addition, a ritual bath in pure water is performed for the dead in many religions including Judaism and Islam. In Islam, the five daily prayers can be done in most cases after completing washing certain parts of the body using clean water (*wudu*). In Shinto, water is used in almost all rituals to cleanse a person or an area (e.g., in the ritual of *misogi*). Water is mentioned in the Bible 442 times in the New International Version and 363 times in the King James Version: 2 Peter 3:5(b) states, "The earth was formed out of water and by water" (NIV).

Some faiths use water especially prepared for religious purposes (holy water in some Christian denominations, *Amrita* in Sikhism and Hinduism). Many religions also consider particular sources or bodies of water to be sacred or at least auspicious; examples include Lourdes in Roman Catholicism, the Jordan River (at least symbolically) in some Christian churches, the Zamzam Well in Islam and the River Ganges (among many others) in Hinduism.

Water is often believed to have spiritual powers. In Celtic mythology, Sulis is the local goddess of thermal springs; in Hinduism, the Ganges is also personified as a goddess, while Saraswati have been referred to as goddess in Vedas. Also water is one of the "panch-tatva"s (basic 5 elements, others including fire, earth, space, air). Alternatively, gods can be patrons of particular springs, rivers, or lakes: for example in Greek and Roman mythology, Peneus was a river god, one of the three thousand Oceanids. In Islam, not only does water give life, but every life is itself made of water: "We made from water every living thing".

The Ancient Greek philosopher Empedocles held that water is one of the four classical elements along with fire, earth and air, and was regarded as the ylem, or basic substance of the universe. Water was considered cold and moist. In the theory of the four bodily humors, water was associated with phlegm. Water was also one of the five elements in traditional Chinese philosophy, along with earth, fire, wood, and metal . Water also plays an important role in literature as a symbol of purification. Examples include the critical importance of a river in *As I Lay Dying* by William Faulkner and the drowning of Ophelia in *Hamlet*.

Sherlock Holmes held that "From a drop of water, a logician could infer the possibility of an Atlantic or a Niagara without having seen or heard of one or the other."

Water is also taken as a role model in some parts of traditional and popular Asian philosophy. James Legge's 1891 translation of the Dao De Jing states "The highest excellence is like (that of) water. The excellence of water appears in its benefiting all things, and in its occupying, without striving (to the contrary), the low place which all men dislike. Hence (its way) is near to (that of) the Tao" and "There is nothing in the world more soft and weak than water, and yet for attacking things that are firm and strong there is nothing that can take precedence of it;--for there is nothing (so effectual) for which it can be changed." Today Bruce Lee is widely quoted "Empty your mind, be formless. Shapeless, like water. If you put water into a cup, it becomes the cup. You put water into a bottle and it becomes the bottle. You put it in a teapot it becomes the teapot. Now, water can flow or it can crash. Be water my friend."

10 . Water portal

Water is described in many terms and contexts:

- **according to state**
  - solid - ice
  - liquid - water
  - gaseous - water vapor

- **according to meteorology**:
  - hydrometeor
    - precipitation

precipitation according to movement

- vertical (falling) precipitation
  - rain
  - freezing rain
  - drizzle
  - freezing drizzle
  - snow
  - snow pellets
  - snow grains
  - ice pellets
  - frozen rain
  - hail
  - ice crystals
- horizontal (seated) precipitation
  - dew

precipitation according to state

- liquid precipitation
  - rain
  - freezing rain
  - drizzle
  - freezing drizzle
  - dew
- solid precipitation
  - snow
  - snow pellets
  - snow grains
  - ice pellets
  - frozen rain
  - hail
  - ice crystals
  - hoarfrost
  - atmospheric

  - hoarfrost
  - atmospheric icing
  - glaze ice

icing

  - glaze ice
- mixed precipitation
  - in temperatures around 0 °C

-
  - levitating particles
    - clouds
    - fog
    - mist
  - ascending particles (drifted by wind)
    - spindrift
    - *stirred snow*
- **according to occurrence**
  - groundwater
  - meltwater
  - meteoric water
  - connate water
  - fresh water
  - surface water
  - mineral water – contains much minerals
  - brackish water
  - dead water – strange phenomenon which can occur when a layer of fresh or brackish water rests on top of denser salt water, without the two layers mixing. It is dangerous for ship traveling.
  - seawater
  - brine
- **according to uses**
  - tap water
  - bottled water
  - drinking water or potable water – useful for everyday drinking, without fouling, it contains balanced minerals that are not harmful to health (see below)

  - purified water, laboratory-grade, analytical-grade or reagent-grade water – water which has been highly purified for specific uses in science or engineering. Often broadly classified as Type I, Type II, or Type III, this category of water includes, but is not limited to the following:
    - distilled water
    - double distilled water
    - deionized water

- **according to other features**
  - soft water – contains less minerals
  - hard water – from underground, contains more minerals
  - distilled water, double distilled water, deionized water - contains no minerals
  - Water of crystallization — water incorporated into crystalline structures
  - Hydrates — water bound into other chemical substances
  - heavy water – made from heavy atoms of hydrogen - deuterium. It is in nature in normal water in very low concentration. It was used in construction of first nuclear reactors.
  - tritiated water

- **according to microbiology**
  - drinking water
  - wastewater
  - stormwater or surface water

- **according to religion**
  - holy water