

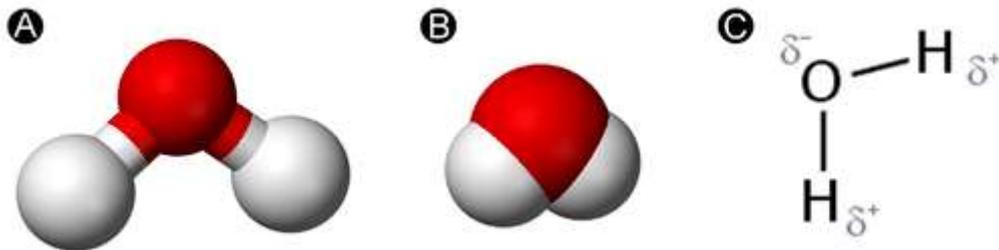
CC-12
UNIT-1
BIOCHEMICAL
FOUNDATIONS
PART-1.2

STRUCTURE OF WATER

Water is a simple molecule consisting of one oxygen atom bonded to two different hydrogen atoms. Because of the higher **electronegativity** of the oxygen atom, the bonds are polar covalent (**polar bonds**). The oxygen atom attracts the shared electrons of the covalent bonds to a significantly greater extent than the hydrogen atoms. As a result, the oxygen atom acquires a partial negative charge (δ^-), while the hydrogen atoms each acquire a partial positive charge (δ^+). The molecule adopts a bent structure because of the two lone pairs of electrons on the oxygen atom.

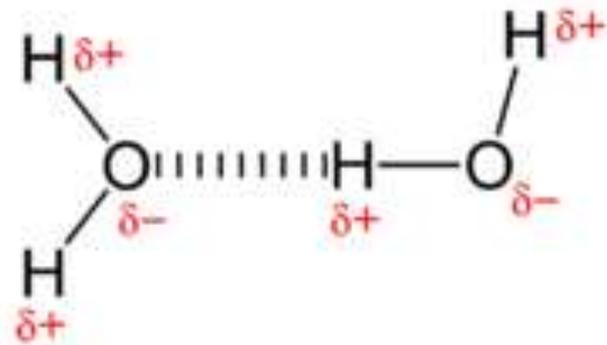
The H–O–H bond angle is about 105° , slightly smaller than the ideal 109.5° of an sp^3 hybridized atomic orbital.

The bent shape of the water molecule is critical because the polar O–H bonds do not cancel one another and the molecule as a whole is polar. The figure below illustrates the net polarity of the water molecule. The oxygen is the negative end of the molecule, while the area between the hydrogen atoms is the positive end of the molecule.



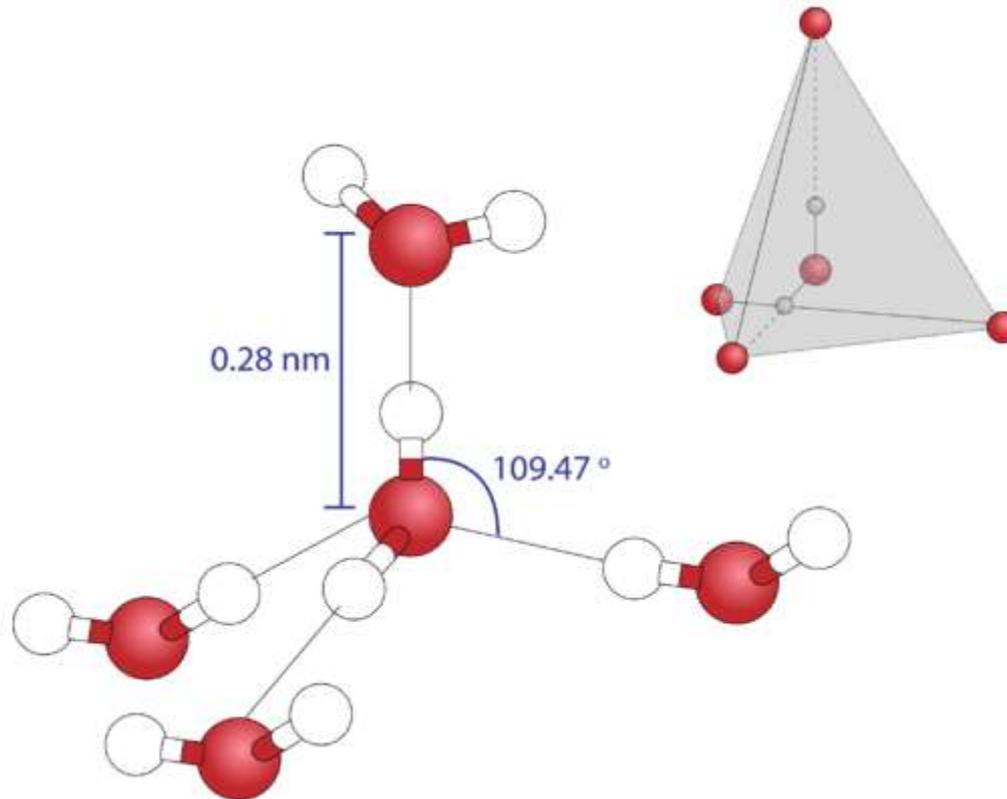
The water molecule, visualized three different ways: ball-and-stick model, space-filling model, and structural formula with partial charges.

Polar molecules attract one another by dipole-dipole forces, as the positive end of one molecule is attracted to the negative end of the nearby molecule. In the case of water, the highly polar O–HO–H bonds results in very little electron density around the hydrogen atoms. Each hydrogen atom is strongly attracted to the lone-pair electrons on an adjacent oxygen atom. These are called hydrogen bonds and are stronger than conventional dipole-dipole forces.



A hydrogen bond is the attraction between a lone pair of electrons on the oxygen atom of one molecule and the electron-deficient hydrogen atom of a nearby molecule.

Because each oxygen atom has two lone pairs, it can make hydrogen bonds to the hydrogen atoms of two separate other molecules. The figure below shows the result—an approximately tetrahedral geometry around each oxygen atom, consisting of two covalent bonds and two hydrogen bonds.



As a result of two covalent bonds and two hydrogen bonds, the geometry around each oxygen atom is approximately tetrahedral.

THE PHYSICAL AND CHEMICAL PROPERTIES OF WATER

Physical Characteristics of Water

Physical properties are reflection of the chemical contents. They have temporal and spatial variations in natural water along two periods. The physical properties of water have a given appearance.

1- Color: Pure water is colorless. Dissolved organic material from decaying vegetation (algae, and humus compounds) and certain inorganic matter for example increasing concentrations of dissolved (Fe and Mn) ions, measured in (ppm) causes color in water. The color is estimated by comparing sample color with a standard solution color (1.245 gm of chloro-platinum potassium added to 1.0 gm of crystalline cobalt chloride in one liter distilled water

2- Odor: released from any water may be due to decreases in the dissolved oxygen (DO₂), presence of organic pollution, and presence of phenols and hydrogen sulfide (H₂S). Pure water is odorless. Quantitative determinations of odor have been developed based on the maximum degree of dilution that can be distinguished from odor-free water.

3- Taste: may be due to increases in the total dissolved solids (TDS), carbonate hardness, decreased dissolved oxygen (DO₂), and excessive bacterial activity, There are no accepted method devised for measuring tastes (Todd, 1980).

All above characteristics are subjective sensation which can be defined only in terms of the experience of a human being.

4- Temperature (ToC): Temperature affects the geochemical and chemical reactions. It effects the acceptability of a number of other inorganic constituents and chemical contaminants that may affect taste. Temperature of groundwater is constant relatively and increases with the depth, it has effects on the hydro geochemical reactions.

5- Turbidity: The turbidity is the measure of suspended and colloidal matter in water such as silt, clay, organic matter and microscopic organisms, also it depend on the structural conditions like flow regime and weathering, and the total suspended solids (TSS). Measurement are often based on the length of the light path passes through the water sample till the image of a flame of a standard candle disappear, turbidity
The physical and chemical properties of water
units is either FT(formazan turbidity units) , or JFU (Jackson turbidity unit). In lakes and rivers it can be measured using Secchi disk method. Ideally, normal turbidity should be below 1 Nephelometric turbidity Unit NTU (WHO, 1997).

6- Hydrogen Ion Concentration (pH): pH is the negative logarithm of hydrogen ion activity and its value expresses the intensity of the activity or alkalinity condition of water under normal condition temperature (T°C) and pressure. Most reactions in gas/water/rock systems involve or are controlled by the pH of the system, it related to taste, and odor problems. PH-value in natural water is affected by the concentration of bicarbonate and carbonate ions. The pH value for all water samples is in the optimum range (6.5-8.5). According to (WHO, 2006), some water samples are described as alkaline water, and the others are close to neutral. The water in a pure state has a neutral (pH=7), while the rain has a natural acidic pH of about 5.6 because it contains CO₂ and SO₂. It measured by pH Electrode meter, or Acidity Index paper.

7- Radioactivity: Water sources can contain radionuclides of natural and artificial origin (i.e. human made). Water may contain radioactive substances (“radionuclides”) that could present a risk to human health.

Radioactivity comes from several naturally occurring elements (including K-40, Ra226, Ra-228, U-234, U-238 and Pb-210), and human-made sources is present throughout the environment such as :radionuclides discharged from nuclear fuel cycle facilities, manufactured radionuclides (produced and used in unsealed form in medicine or industry) entered into drinking-water supplies as a result of regular or incidental discharges, and radionuclides released in the past into the environment, including drinking water sources. Some chemical elements present in the environment are naturally radioactive. Earth is constantly bombarded by highenergy particles originating both from the sun and from outside the solar system. Collectively, these particles are referred to as cosmic radiation. Everybody receives a dose from cosmic radiation, which is influenced by latitude, longitude and height above sea level.

Chemical properties of water

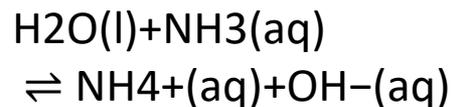
Water reacts with a lot of substances to form different compounds. Some significant reactions are as follows:

1. Amphoteric nature:

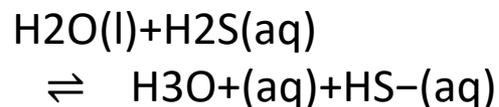
Water can act as both acid and base, which means that it is amphoteric in nature.

Example:

Acidic Behaviour:

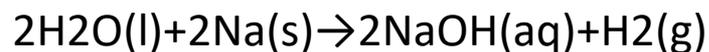


Basic Behavior:



2. Redox reactions:

Electropositive elements reduce water to hydrogen molecule. Thus, water is a great source of hydrogen. Let us see an example in this case:



During the process of photosynthesis, water is oxidized to O_2 . As water can be oxidized and reduced, it is very useful in redox reactions.

3. Hydrolysis reaction

Water has a very strong hydrating tendency due to its dielectric constant. It dissolves many ionic compounds. Some covalent and ionic compounds can be hydrolyzed in water.

Chemical Characteristics of Water

Chemical formula: H₂O

Molar mass: 18.01528(33) g/mol

Density

Solid: 0.9167 g/ml at 0 °C

Liquid: 0.961893 g/mL at 95 °C

0.9970474 g/mL at 25 °C

0.9998396 g/mL at 0 °C

Boiling point: 99.98 °C (211.96 °F; 373.13 K)

Melting point: 0.00 °C (32.00 °F; 273.15 K)

Solubility: Poorly soluble in aliphatic and aromatic hydrocarbons, and Ethers.

Improved solubility in amines, ketones, alcohols, carboxylates.

Miscible with acetonitrile, dimethyl sulfoxide, dimethoxyethane, dimethylformamide, acetaldehyde, sulfonates, tetrahydrofuran, 1,4-dioxane, glycerol, acetone, isopropanol, propanol, ethanol, methanol.

Partially miscible with Bromine, Ethyl Acetate, Diethyl ether, Dichloromethane.

Acidity (pKa) : 13.995

Vapour pressure: 3.1690 kilopascals or 0.031276 atm

Basicity (pKb): 13.995

Refractive index(nD) : 1.3330 (20°C)

Thermal conductivity	0.6065 W/m·K
Viscosity	0.890 cP
<u>Structure</u>	
Crystal structure	Hexagonal
Molecular shape	Bent
Point group	C_{2v}
Dipole moment	1.8546 D
<u>Thermochemistry</u>	
Specific heat capacity (C)	75.375 ± 0.05 J/mol·K
Std enthalpy of formation ($\Delta_f H^\circ_{298}$)	-285.83 ± 0.040 kJ/mol
Std molar entropy (S°_{298})	69.95 ± 0.03 J/mol·K
Gibbs free energy ($\Delta_f G^\circ$)	-237.24 kJ/mol