

## REVIEW ARTICLE

WATER (H<sub>2</sub>O) AT GLANCE

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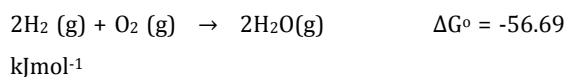
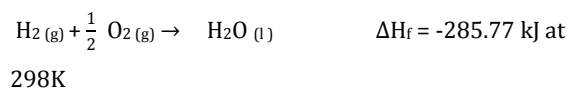
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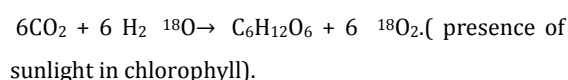
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On earth planet surface 70% water, out of which 3% water useful for drinking and other purposes. 1% water is easily available.

The Water is formed from two hydrogen atoms and one oxygen atom.

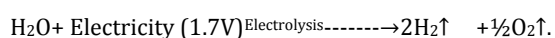


Water is more valuable than platinum and gold metals. Human being and living organisms not survive and sustain their life without water. Ordinary water used as coolants in nuclear power reactor. The mechanism of photosynthesis has been studied using <sup>18</sup>O isotope in water. Using <sup>18</sup>O it has been shown that the oxygen released in photosynthesis is not from CO<sub>2</sub> but from water.



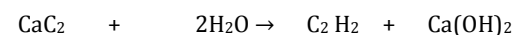
The potential energy of water is converted into electricity at hydropower station. Steam produced from water by atomic energy. Pressurized steam sent to turbine and generator generates electricity. Steam is produced from water at geothermal stations also for electricity.

In future Hydrogen is fuel. The Hydrogen is clean, non polluted energy source, obtained from electrolysis of water.



During electrolysis process the hydrogen is evolved at cathode and oxygen at anode.

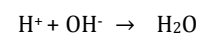
Water will be produces **combustible gases** with some chemicals e.g. Acetylene gas is obtained from CaC<sub>2</sub>.



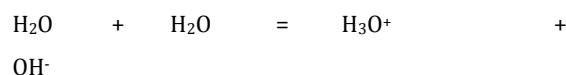
Calcium carbide water Acetylene Calcium hydroxide

Combustion of acetylene produces 310.4 calories of energy.

Neutralization, in general, is the combination of H<sup>+</sup> ions of an acid with OH<sup>-</sup> ions of a base to form the practically unionized water.



Acid-base neutralization reactions taking place in water. (water system concept)



Acid 1                  Base 2                  Acid 2 (conjugate acid to base 2)          Base 1 (Conjugate base to acid 1)

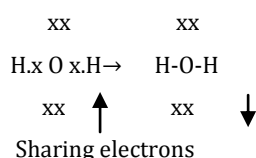
Hydration energy released when one mole of gaseous cation is plunged into water. Hydration of positively charged cation is an electrostatic phenomenon, both the charge on the cation (Z) and radius of cation (r) contribute to the value of hydrogen energy.  $\Delta H_{\text{hyd}}$  for Cs<sup>+</sup> is -263 kJmol<sup>-1</sup>, for Fe<sup>3+</sup> is -4376 kJ mol<sup>-1</sup>, for Na<sup>+</sup> is -405 kJmol<sup>-1</sup>.  $\Delta H_{\text{hyd}}$  decreases, pK<sub>a</sub> values increases. Higher the  $\Delta H_{\text{hyd}}$ , lower is the pK<sub>a</sub> and higher is the acidity. pK<sub>a</sub> value of Na<sup>+</sup> is 14.5, of Fe<sup>3+</sup> is 2.2, of Ti<sup>4+</sup> is -4.0.

In H<sub>2</sub>O molecule two hydrogen atoms are covalently bonded to the highly electronegative Oxygen atom. Here each H atoms can hydrogen bond to the Oxygen atom of another molecule, thus forming large chains or cluster of water molecules. Each Oxygen atom has unshared electron pair which leads

to hydrogen bonding with other water molecule. Thus Liquid water is made of cluster of a large number of molecules. Oxygen atom (2,6) has six valence electrons and can achieve the stable octet by sharing two electrons, one with each H atom.

Thus Lewis Structure of water can be written as

Unshared electron pair



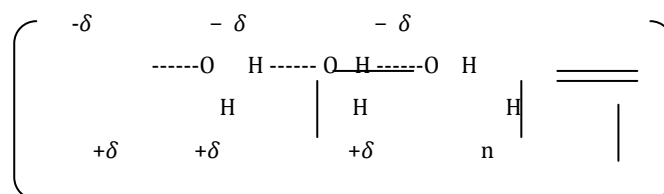
Water is one component System. Three phase equilibria exist, Solid Ice = Liquid Water, Liquid Water = Water Vapour, Solid Ice = Water Vapour. The phase co exists at triple point.

At temperature higher than critical point, liquid – Vapour equilibria do not occur, only vapour phase exists. Critical Point Temperature 374°C (647K) Pressure 223 bar OR 218 atm, Triple Point Temp: 0.0098 °C (273.0098K) [273.0075K : F.P + 273.0023K : M.P]. Boiling Point temperature 100°C Cat Pressure 1.013bar OR 1 atm.

Tritium isotope occurs in very small quantities in nature. Out of  $10^{10}$  parts in ordinary water only 7 parts are tritium. It is also found in heavy water ( $\text{D}_2\text{O}$ ). When the volume of 75 tons of water after being electrolyzed reduces to mere 0.5  $\text{cm}^3$ . It is shown by mass spectrograph that in  $10^4$  parts of it only 1 part of tritium is present.

Water is hydride group 16 elements, Oxygen. Oxygen is highly electronegative element. Due to large difference in electronegativity between the two atoms (Hydrogen and Oxygen) water behaves as dipoles i.e.  $\text{H}\delta^+ - \text{H}\delta^-$ .  $\text{H}\delta^- - \text{H}\delta^+$  bonds become highly polar. Polar molecules interact strongly with other dipoles. When these two dipoles are brought closer

(dipole-dipole attraction), they will be linked together by a special type of bond called **hydrogen bond**. Hydrogen atom acts as a bridge between the two strongly electronegative atoms, holding one by a covalent bond and the other by purely electrostatic forces.



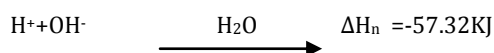
Hydrogen bond is stronger than van der Waals forces of attraction but weaker than covalent bonding.  $\text{H}_2\text{O}$  molecules get associated due to intermolecular hydrogen bonding. They form associated molecules or Clusters  $(\text{H}_2\text{O})_n$ . Water exists as a liquid  $(\text{H}_2\text{O})_n$  liquids whose molecules are held together by hydrogen bonds are called associated liquids. Polywater have freezing point  $-40^\circ\text{C}$  and a very high density of  $1.4 \text{ gm cm}^{-3}$ , enthalpy of formation  $-120 \text{ kJ mol}^{-1}$ . In ice, each water molecule is tetrahedrally associated with four water molecules due to Hydrogen bonding. Association is responsible for the abnormally high B.P. & M.P. of water. Greater the dielectric constant of solvent, greater is its dissociating power, water has greater dielectric constant Value 78.4 then it behaves good ionizing solvent.

In general like dissolves like, e.g. ionic salts or ionic solute (polar solute) dissolve more readily in polar solvent like water than non-polar solvent like alcohol, benzene & carbon tetrachloride. Energy required to separate inorganic compounds/solids (Lattice energy) is obtained from polar solvents having high dielectric constant, most of the ionic compounds dissolve in water. The cations and anions get hydrated (solvated) and then dissolve.

Table 1: General information about the water molecule

1.	Molecular formula	:	H <sub>2</sub> O
2.	Molecular shape	:	Angular
3.	Mole. Wt.	:	18
4.	Boiling point	:	100°C.
5.	Melting Point	:	0°C
6.	Ice point	:	273.15 K
7.	Density Maximum Density	:	0.997073gm cm <sup>3</sup> at 25°C 1 at 4°C
8.	Refractive index	:	1.33254
9.	Surface tension	:	71.97 dyne cm <sup>-1</sup>
10.	Viscosity	:	0.8937 centipoise
11.	Dissociation Temperature	:	2000°C
12.	Vapour Pressure	:	23.756 mm of Hg
13.	Equilibrium Constant	:	1.04 x10 <sup>-14</sup>
14.	Dielectric Constant	:	78.4 to 81.1
15.	ΔH Formation	:	-285.8 kJ mol <sup>-1</sup> at 298K or -242 kJ mol <sup>-1</sup>
16.	enthalpy charge ΔH <sup>o</sup>	:	-229.9kJ mol <sup>-1</sup> (H <sup>+</sup> =0.0 , OH <sup>-</sup> =-229.9)
17.	ΔS (entropy change)	:	69.9 Joule mol <sup>-1</sup> K <sup>-1</sup>
18.	ΔG (Free energy change)	:	-237.2 KJ mol <sup>-1</sup> at25°C and 1atm
19.	ΔG <sup>o</sup>	:	-56.69 KJ mol <sup>-1</sup>
20.	Dipole moment (μ <sub>obs</sub> )	:	1.82 Debye or 1.84 D or 1.85 Debye
21.	μ <sub>OH</sub>	:	1.52Debyes
22.	H-O-H angle	:	105° or 104.5° or 104°5' or 104°28'
23.	O-H bondlength	:	0.96Å or 0.96x10 <sup>-10</sup> m
24.	Bond energy H-O-H	:	118 kcal mol <sup>-1</sup> or 29.29 kJ mol <sup>-1</sup>
25.	Hydrogen bond, bond energy Strength of hydrogen bond	:	2 to 10 kcal mol <sup>-1</sup> About 20 kJ mol <sup>-1</sup>
26.	Symmetry	:	C <sub>2</sub> V
27.	Mobility H <sup>+</sup> Mobility OH <sup>-</sup>	:	36.25x10 <sup>-8</sup> m <sup>2</sup> v <sup>-1</sup> s <sup>-1</sup> 20.64x10 <sup>-8</sup> m <sup>2</sup> v <sup>-1</sup> s <sup>-1</sup>
28.	Magnetic Susceptibility	:	- 89x10 <sup>-6</sup>
29.	Molar Magnetic Susceptibility	:	-1.60 x 10 <sup>-3</sup> ml

The oppositely charged particles can coexist in water; therefore it is a good ionizing medium. This increases the chemical reactions.



The relative orientation of water molecules is more favorable in ice because of the ordered hydrogen-bonded networks. Electrical conduction studies show that mobility of the H<sup>+</sup> ion is nearly 50

times higher in ice than in liquid water. Both H<sup>+</sup> and OH<sup>-</sup> ions have significantly greater mobility than the other ions. If H<sup>+</sup> and OH<sup>-</sup> ions moved as clusters, their mobility would be less than those of the other ions.

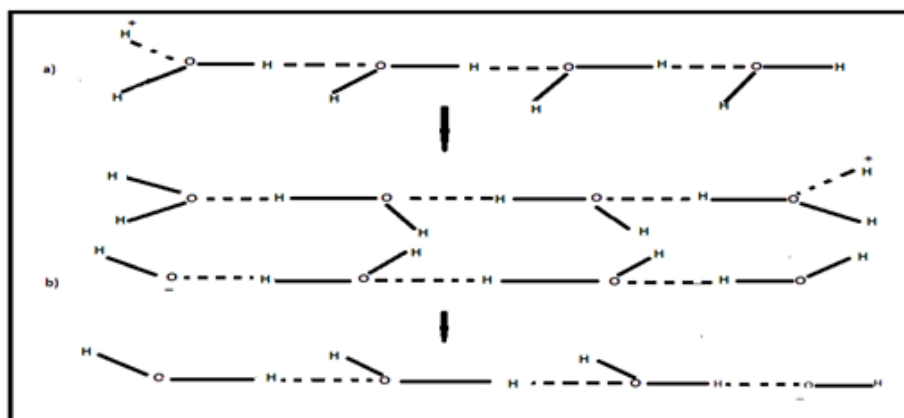
The high mobility observed is attributed to the chain mechanism. The ability of H<sup>+</sup> and OH<sup>-</sup> ions to move along water molecules joined through hydrogen bonds. Since the rigid hydrogen bonded

structure of the ice should facilitate efficient Proton transfer.

It has been suggested that tunneling also plays a role in proton transfer reaction. Wavelike

behavior allows particle to pass through potential barriers, the effect of tunneling is equivalent to reducing the activation energy and thus increasing the rate.

#### A Chain mechanism for the transfer of (a) H<sup>+</sup> and (b) OH<sup>-</sup> across water molecules.



Water is strong dipole. It can polarize of noble gas atoms and due to attraction between dipole water and induced dipole-noble gas atom, hydrates are obtained. The gases Ar, Kr and Xe forms gas hydrates Ar. 5 H<sub>2</sub>O, Kr.5 H<sub>2</sub>O, Xe.6H<sub>2</sub>O, Kr.5 D<sub>2</sub>O, Xe.6D<sub>2</sub>O. Solids that consist of molecules of a compound together with water molecules are called hydrates eg. ScCl<sub>3</sub>. 6 H<sub>2</sub>O. The gases Ar, Kr and Xe may be trapped in cavities of water when water solidifies. The compounds inert gas hydrates have formulae approximately to 6 H<sub>2</sub>O:1 gas atom. The hydrates of noble gases prepared by bringing vapours of water and noble gas together under Pressure at low temperature. They are crystalline compounds.

#### Liquid hydrates:

Chloroform and ethyl chloride has unitcell containing 136 water molecules with 8 large cages and 16 smaller ones. The anesthetic effect of substance such as chloroform may be due to the formation of liquid hydrate crystals in brain tissue.

#### Salt hydrate:

It is formed when tetraalkylammonium or sulfonium salts crystalline from aqueous solution with high water content eg. [(C<sub>4</sub>H<sub>9</sub>)<sub>4</sub>N]C<sub>6</sub> H<sub>5</sub>CO<sub>2</sub>.39.5 H<sub>2</sub>O OR [(C<sub>4</sub>H<sub>9</sub>)<sub>3</sub>S]F.20H<sub>2</sub>O

Water exchange in Aqua Ions [M(H<sub>2</sub>O)<sub>n</sub>]<sup>m+</sup>

Water exchange reactions in which five typically inert aqua ions M= Cr<sup>3+</sup>, Co<sup>3+</sup>, Rh<sup>3+</sup>, Ir<sup>3+</sup> and Pt<sup>2+</sup>. Have exchange rate constant in the range 10<sup>-3</sup>-10<sup>-6</sup> s<sup>-1</sup>. Water exchange is characteristically slow.

#### Structure of Water molecule:

Water molecule is a non-linear (Geometry), triatomic molecule with a bent structure and it possesses permanent dipole moment.

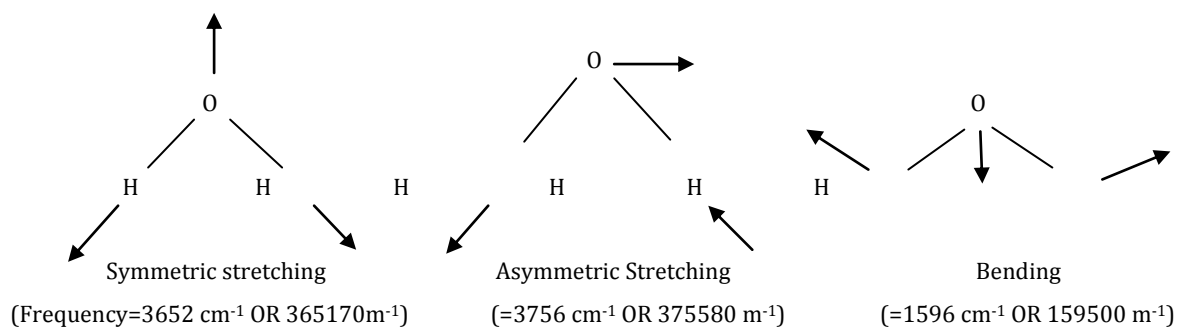
In a vibration of spectrum of a molecule we are concerned with the number of fundamental vibrational modes of a molecule. Each fundamental mode corresponds to a band in spectrum and each vibrational degree of freedom corresponds to the fundamental mode of vibration. Total degrees of freedom for a molecule with 'n' atoms are 3n (3x3=9). 3n degrees of freedom = Rotational + Translational + Vibrational. Vibrational=3n degrees of freedom - (Rotational + Translational)

For non-linear molecule having 'n' number of atoms, show three translational & three rotational degrees of freedom. Therefore, the expression for vibrational degrees of freedom will be given by 3n - (3+3)=3n-6.

Degree of vibrational freedom = 3x3-6=9-6=3, Where n=3, three atoms in water. Water molecule shows three modes of vibration two are stretching vibration

& one bending vibration. All these vibrations involve change in dipole moment ( $\mu \neq 0$ ) Hence all the three

modes will be IR active.



**Then normal modes of vibration of water molecule:**

For water molecule that does not possess center of symmetry and has permanent dipole

moment. All the vibrational modes of water molecule are Raman as well as IR active.

Vibrational modes of water

Mode of Vibration	Symmetric stretching	Asymmetric stretching	Bending
IR	Active	Active	Active
Raman	Active	Active	Active

#### Spectrum for H<sub>2</sub>O Molecule:

- Symmetric stretching: Dipole moment changes, IR active. Polarizability changes, Raman active; produce intense Raman lines.
- Asymmetric stretching: Dipole moment changes, IR active. Polarizability changes, Raman active. However the change in polarization is very small and Raman lines are very weak.
- Symmetric bending: Dipole moment changes to some extent hence IR active. Change in Polarizability is very small hence Raman absorption is unobservable, gives unobservable lines.

The Symmetries of the molecular orbitals of the H<sub>2</sub>O molecule derived from the 2s and 2p orbitals of the O atom and the 1s orbitals of the two H atoms.

In case H<sub>2</sub>O molecule, there are two vertical planes of symmetry one is given the label  $\sigma_v$  and the other  $\sigma'_v$ . Water molecule has a twofold axis of rotation denoted by  $C_2$ . The H<sub>2</sub>O molecule has the symmetry elements E,  $C_2$ ,  $\sigma_v$  and  $\sigma'_v$  (Set of symmetry operations together – Point groups).

#### Why drink water?

Water helps to lose weight, maintains healthy heart & healthy skin, fights infections, get rid of body toxins, prevent joint pains and arthritis, Boost eyes, Prevent constipation, Reduce risk of Cancer. Improves Productivity etc. According to age everyday 1.5 to 5 liter pure drinking water (Oxygenated water: 14 ppm) essential for human body. Water is elixir of life. Water is the large constituent of the body. The average body water is 60 to 70 percent of the total body weight. Females contain a little less amount of water than males. Water has the highest latent heat evaporation than any other liquid. A Certain amount of water can cause maximum cooling by evaporation; so that the body temperature does not rise. Water can form true solutions as well as colloidal solutions. Even the water insoluble substances are made water soluble by the hydrotropic action. Therefore it is most suitable solvent for cellular components; water thus brings various substances in contact for chemical reactions to proceed. A large number of chemical reactions in the body are accelerated by water

(catalytic action) due to its ionizing power. All chemical reactions in the body proceed in presence of water only. Water acts as a lubricant in the body to

prevent friction in joints, pleura, conjunctiva and peritoneum.

**Control Pollution, Save Water and Save Planet.**

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