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Role of Water in Chemical Reaction and Chemistry of Water

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ABSTRACT

As a ubiquitous solvent and an active ingredient in numerous biochemical and medicinal processes, water is essential to chemical reactions. Water helps drug molecules dissolve, hydrolyse, and ionise, which affects the drugs' bioavailability and therapeutic effectiveness in pharmaceutical sciences. It serves as a reaction medium that promotes molecular collisions, stabilises transition states, and permits appropriate reactant mixing. Additionally, water directly takes part in enzymatic transformations, oxidation-reduction, hydrolysis, and other chemical events that are essential to drug metabolism. It is also essential for formulation development, buffer preparation, and quality control procedures due to its polarity and hydrogen-bonding ability. Therefore, it is crucial to comprehend how water functions in chemical reactions in order to create stable medication products, maximise reaction yields, and guarantee patient safety.

KEYWORDS: Universal solvent, catalyst, amphoteric nature, hydrogen bonding, autoionization, hydrolysis, reaction medium, proton donor/acceptor.

INTRODUCTION

Water is essential to all life on Earth, and when there is a shortage, such as due to extremes in temperature, unique coping mechanisms are required. With significant ramifications for forecasts regarding the probability of habitable conditions, this circumstance has strengthened the widely held belief that water is a necessary condition for life in the cosmos as a whole. However, until we fully comprehend the role that water does play in supporting terrestrial life, we are unable to evaluate that assertion. For instance, driving hydrophobic interactions and their sensitivity to tiny solutes, aiding proton transport, influencing protein-protein and receptor-substrate interactions, serving as a reagent in biological activities, and adjusting electronic excitation energies. Everyone agrees that water is vital to life and an important mediator for chemical processes. It is a flexible participant in chemical and biological processes due to its distinct physicochemical characteristics, which include polarity, hydrogen bonding ability, high dielectric constant, and amphoteric nature. In aquatic settings, many medication compounds hydrolyse, which affects their stability, bioavailability, and shelf life. In the human body, water is involved in enzymatic reactions, hydration, condensation, and redox activities as well as acid-base reactions. Water is utilised in formulation science to create solutions, suspensions, and emulsions, which have an impact on medication solubility and therapeutic effectiveness. Additionally, it is essential for parenteral preparations, reconstitution of lyophilised goods, and dissolution tests. The components that make up water have a big impact on its characteristics. Despite the fact that water is necessary for life on Earth, some of its components may make it unfit for both industrial and human consumption. To design suitable treatment systems for the use of water in different applications, proper characterization is required.

THE UNIQUENESS OF WATER

The ability of water to build three-dimensional networks of molecules that are hydrogen bound to one another makes it unique among liquids (5, 7, 30, 34, 41, 43, 115, 124). This is because every water molecule contains four fractional charges that are orientated towards the corners of a typical tetrahedron in three dimensions. Two of these are negative (the oxygen atom's lone pairs of electrons) and two are positive (the hydrogen atoms). Each water molecule can form up to four weak interactions (hydrogen bonds) with nearby water molecules as a result of this distribution of positive and negative poles, with one molecule's positive pole being drawn to another's negative pole. Figure 1 shows a two-dimensional projection of the crystal structure of ice. Every water molecule in this instance has four hydrogen connections with other atoms, and all of these hydrogen bonds are linear, meaning that every hydrogen atom is covalently bound to one atom and hydrogen bonded to the other atom, forming a straight line between the two O atoms. These are strong straight bonds. Ice is distinguished by its incredibly open structure (it has a density of 0.92 at 0°C).

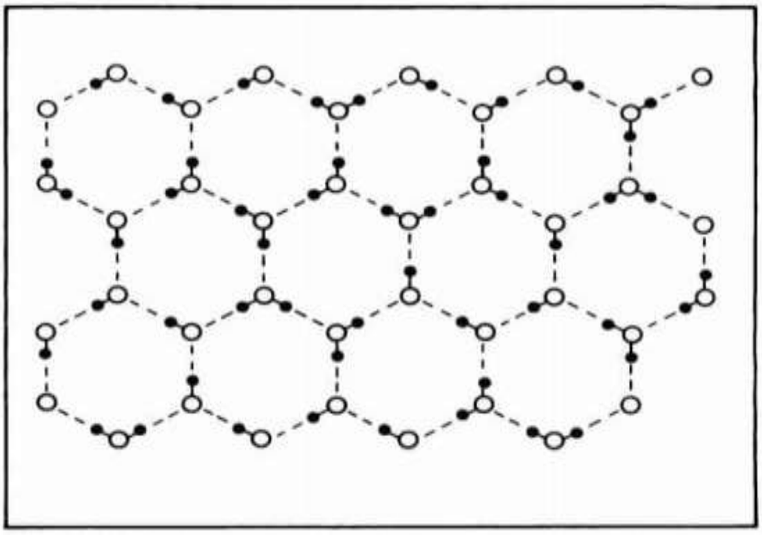

Fig 1Two-dimensional projection of the crystal structure of ice.

Certain hydrogen bonds are disrupted when ice melts, allowing molecules to enter the vacant spaces and create the denser (around 1.0) liquid water. The most significant characteristic of liquid water for the purposes of this article is that its molecules are now too close to one another to form many of the strong, straight hydrogen bonds that defined ice.There aren't many hydrogen atoms that align perfectly with oxygen atoms, and the bending bonds that do develop are not very strong.Water is a somewhat liquid, thus even though hydrogen bonding is still present throughout the liquid (7), the bonds' fragility permits the structure to be broken.

REACTIONS IN WATER

Water and other unconventional solvents are becoming more popular as a result of the increased demand for more environmentally friendly methods in chemical synthesis. Water is the most readily available and least expensive solvent to utilize in a process. It is harmless and nonflammable, and it may separate organic substrates through straightforward phase separation when a biphasic reaction system is employed. In addition to having the highest specific heat capacity, which makes it easier to manage an exothermic reaction, water also has a network of hydrogen bonds that can affect the reactivity of substrates.9. Additional intriguing characteristics of water include the ability to use cosolvents or biphasic reaction systems, add additives like salts, which can cause salting-in or salting-out effects, or add surfactants and cyclodextrins. The pH can also be changed.

Despite these special qualities, water has not historically been the preferred solvent for conducting chemical processes. One explanation for this has been that organic synthesis methods frequently call for the employment of water-sensitive catalysts, reagents, or intermediates, and that organic molecules' nonpolarity causes them to be poorly or completely soluble in water.

Isolating materials that are soluble in water might also present challenges. However, over the last 20 to 30 years, the potential advantages of employing aqueous media have been acknowledged, and reactions such as Michael additions, organometallic reactions, and pericyclic reactions have been documented. In certain instances, water has also boosted the reaction rate and selectivity.

The Diels-Alder reaction, which produces multiple distinct stereocenters in a single step, is one of the most extensively researched reactions in water.5–9, 14 Breslow emphasised the rate improvements seen in water for the reaction between cyclopentadiene and butanone in the 1980s, despite the fact that Diels-Alder reactions were first documented in aqueous environments in the 1930s (1).16 It's interesting to note that the reaction rate in methanol was comparable to that of other organic solvents, whereas the unexpected acceleration in water was ascribed to hydrogen bonding and enforced hydrophobic interactions.16, 17 Additional research demonstrated that employing water as a solvent can result in improved endo/exo (N/X, 2a/2b) product ratios. For example, when cyclopentadiene was used as the solvent, the N/X ratio was roughly 4, but this was raised to over 21 in water.

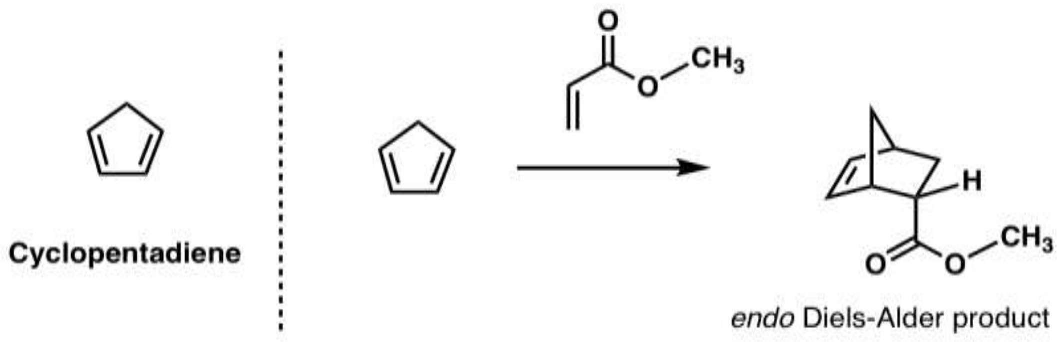

Fig 2 Diels-Alder reaction between cyclopentadiene and butan-2-one in solvents including water

WATER AS A SOLVENT

It is commonly acknowledged that of these three types, electrostatic and solvophobic interactions are most sensitive to the solvent. Water and other polar liquids work well as solvents for polar or ionic substances. For instance, ionic materials have a broad variety of functionality due to their ability to dissolve and dissociate into ionic fragments. In nonpolar fluids like liquid methane, these options are restricted. The strength of electrostatic interactions between ions in polar liquids is inversely proportional to the solvent dielectric constant when compared to the cases of gas phase or nonpolar solvents. As a result, those ionic contacts may become stronger than other non-covalent interactions. For protein folding and aggregation, as well as the self-organization of cell walls. The hydrophobic effect's peculiar temperature dependence is one of its defining characteristics; unlike electrostatic and van der Waals interactions, it frequently gets stronger with temperature, peaking above 60°C. The cold denaturation of proteins, which occurs when proteins lose their natural structure when cooled, is a particularly fascinating illustration of the hydrophobic effect's inverse temperature dependence (Privalov 1990).

WATER AS CATALYST

In a variety of chemical and biological processes, water can serve as a catalyst. By giving or receiving protons, promoting bond formation or cleavage, and stabilizing transition states through hydrogen bonding, it momentarily contributes to the chemical mechanism. Water is a real catalyst since, crucially, it is regenerated at the conclusion of the reaction rather being consumed. Here fig 3 represents an example of water act as an catalyst in ester hydrolysis.

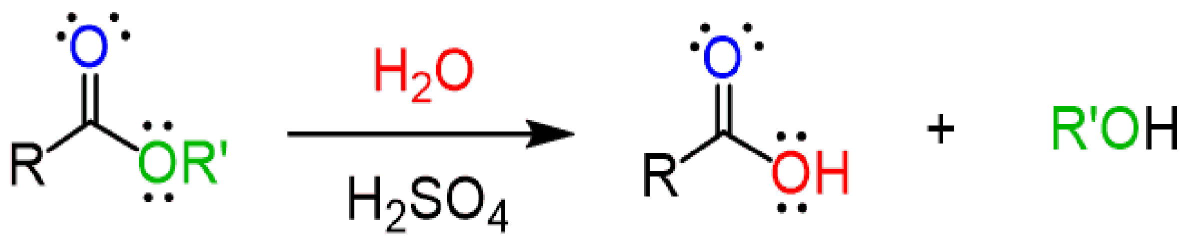

Fig 3 Ester Hydrolysis.

WATER AT ELEVATED TEMPERATURE(WET)

In reaction processes, water at elevated temperatures (WET) can function as a catalyst, solvent, and reactant all at once. WET has been effectively used to remove protective groups, reducing the requirement for additional strong acids or bases, neutralization, and waste salt removal. For several model aryl compounds, procedures are provided for the water-mediated removal of a number of typical protective groups, including tert-butyl carbamates (N-Boc) from 125 to 150 °C, acetamide (N-Ac) at 275 °C, and acetate esters (O-Ac) at 250 °C. Furthermore, it is shown that merely adjusting the temperature can provide high yields and selectively deprotect one protective group in the presence of another.

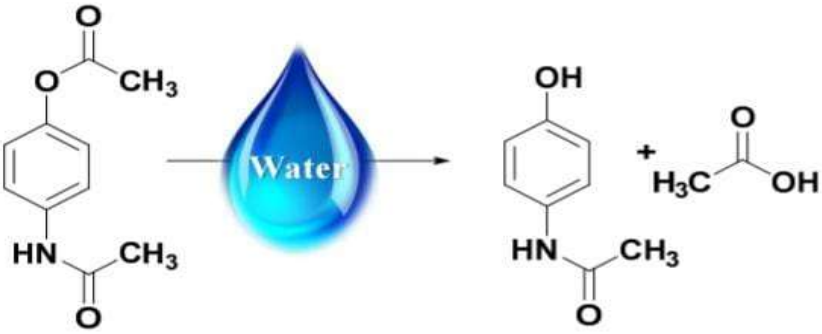

Fig 4 WET as reactant, catalyst and solvent.

WATER IN RADICAL REACTION

Reactions "on water" occur in aqueous suspensions and include organic compounds that are insoluble in water [8,9,10,11,12]. Because of their excellent efficiency and applicability in simple synthetic methods, they have drawn a lot of interest. Examples of free radical chemistry that are helpful for organic synthesis that takes place in a heterogeneous phase will be provided in this section. We will specifically look at (i) "on-water" reactions where the reactants are not soluble in water and (ii) "in-and-on-water" reactions where the radical reactivity is transferred by an amphiphilic co-reactant with some reactants soluble in water and others suspended.

Several groups have developed trifluoromethylation based on radical intermediates in water or aqueous medium; it has excellent functional group tolerance and works broadly on a range of substrates [63,64,65,66]. These results are predicated on the discovery of a generic process that, as illustrated in Figure 5, combines tert-butyl hydroperoxide (TBHP), CF3SO2Na (sometimes referred to as the Langlois reagent), and catalytic quantities of metal catalyst to produce a CF3• radical. The method's optimization demonstrates that catalysts such as FeSO4 or CuSO4 in CH2Cl2/H2O (2.5:1) function effectively, although the trace metals present in the reagents were also enough. Comparable outcomes have been noted for the system that uses water as the only solvent.

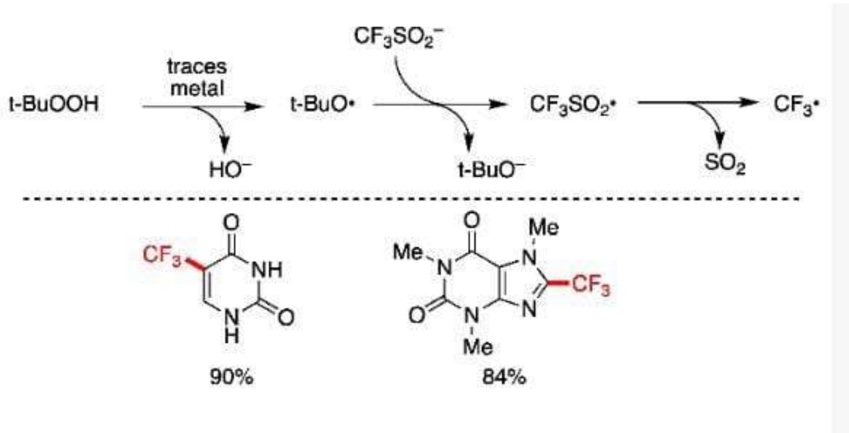

Fig 5 Copper-catalyzed trifluoromethylation using CF_3SO_2Na: (**a**) the mechanism of $CF_3^{\bullet}$ generation from CF_3SO_2Na and tert-butyl hydroperoxide (TBHP).

CHEMISTRY OF WATER

Water is a material that exists in gassy, liquid, and solid phases and is made up of the chemical factors hydrogen and oxygen. It's among the most common and necessary substances. At room temperature, it's an odourless and tasteless liquid with the pivotal capacity to dissolve a wide range of other composites. Indeed, living effects depend on water's rigidity as a detergent. Living effects calculate on waterless results, similar blood and digestive authorities, for natural functions, and it's allowed that life first surfaced in the waterless results of the world's swell. Water seems colourless in small quantities, but it actually possesses an essential blue shade due to a minor immersion of red wavelength light.

Despite having a simple structure (H2O), water molecules have incredibly complex physical and chemical characteristics that are not typical of most other substances on Earth. For instance, while it is typical to see ice cubes floating in a glass of ice water, this type of activity is uncommon for chemical entities. Since the solid state of practically all chemical compounds is denser than the liquid state, the solid would sink to the bottom of the liquid. Since the ice that forms on ponds and lakes in colder parts of the world serves as an insulating barrier to protect the aquatic life below, the ability of ice to float over water is extremely significant in the natural world. Water is the substance with chemical formula H20,one molecule of water has 2 hydrogen atoms covalently bonded to a single oxygen atom as illustrated in fig 6.

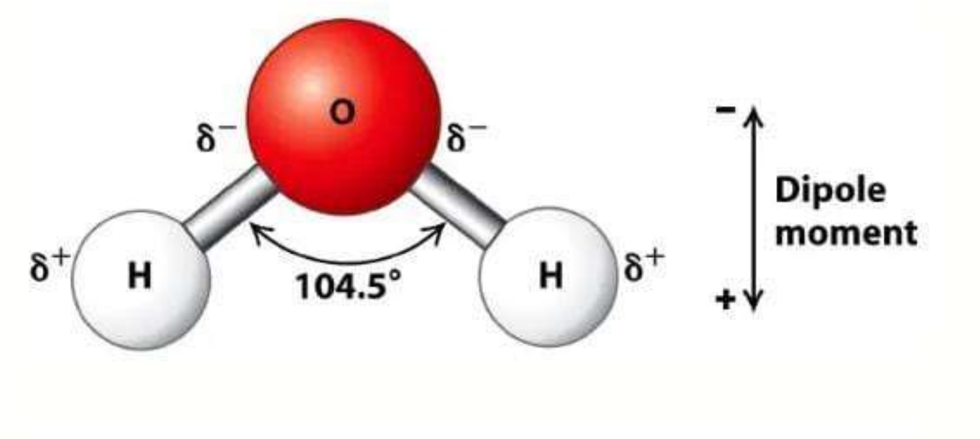

Fig 6 water molecule

HYDROGEN BONDING

The process of hydrogen bonding in water is the attraction of one water molecule's slightly positive hydrogen atoms to another water molecule's slightly negative oxygen atoms, creating a dipole-dipole interaction. These weak yet many associations are always forming and breaking in liquid water, giving it characteristics like cohesiveness and a higher boiling point. Ice is less dense than liquid water because of these linkages, which create a solid, open crystalline structure in which each molecule is connected to four others**.**

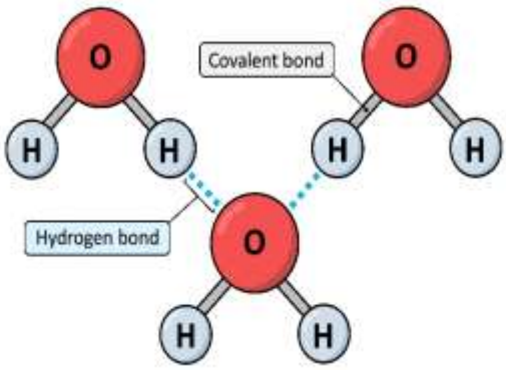

Fig 7 Hydrogen bond in water.

OXYGEN BONDING

Because of its stronger electronegativity, oxygen pulls the participated electrons closer to the hydrogen tittles to form two polar covalent bonds, giving the hydrogen tittles a partial positive charge and oxygen a partial negative charge. Water is a polar patch due to this uneven sharing, and a weaker but essential hydrogen bond is formed when the incompletely positive hydrogen of one water patch is attracted to the incompletely negative oxygen of another.

CONCLUSION

In addition to being a common solvent, water actively participates in and catalyzes a variety of chemical and biological activities. It can stabilize reactants, minimize activation energy, and aid in processes like hydrolysis, hydration, and redox reactions thanks to its special chemical characteristics, which include polarity, hydrogen bonding ability, and amphoteric nature. Water is therefore an essential medium for life and chemistry since it is essential to maintaining chemical reactions in industry, living systems, and nature. In many processes, water serves as both a solvent and a catalyst because of its polarity, hydrogen bonding, and amphoteric nature. It is necessary for chemical, industrial, and biological systems because it facilitates hydrolysis, hydration, and other activities.

REFERENCES

1. Wiggins, P. M. (1990). Role of water in some biological processes. *Microbiological Reviews*, *54*(4), 432-449.

2. *Manna, A., & Kumar, A. (2013). Why does water accelerate organic reactions under heterogeneous condition?. The Journal of Physical Chemistry A, 117(12), 2446-2454.*
3. *Reynolds, W. L., & Lumry, R. W. (1955). Role of Water in Oxidation-Reduction Reactions. The Journal of Chemical Physics, 23(12), 2460-2461.*
4. *Vohringer-Martinez, E., Hansmann, B., Hernandez, H., Francisco, J. S., Troe, J., & Abel, B. (2007). Water catalysis of a radical-molecule gas-phase reaction. Science, 315(5811), 497-501.*
5. *Li, C. J., & Chen, L. (2006). Organic chemistry in water. Chemical Society Reviews, 35(1), 68-82.*
6. *Maréchal, Y. (2006). The hydrogen bond and the water molecule: The physics and chemistry of water, aqueous and bio-media. Elsevier.*
7. *Akiya, N., & Savage, P. E. (2002). Roles of water for chemical reactions in high-temperature water. Chemical reviews, 102(8), 2725-2750.*
8. *Garrett, B. C., Dixon, D. A., Camaioni, D. M., Chipman, D. M., Johnson, M. A., Jonah, C. D., ... & Zwier, T. S. (2004). Role of water in electron-initiated processes and radical chemistry: Issues and scientific advances. Chemical reviews, 105(1), 355-390.*