

VI. MAN AND BIOSPHERE

RESEARCH ON THE ALPHA OMEGA WATER® CRYSTAL INSTRUMENT: RESULTS AND ANALYSES WITH FT-IR, EIS, NMR, AND DFT

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Abstract: Alpha Omega Water® represents an innovative approach within environmental engineering aimed at improving the physicochemical properties of water as a key natural resource. As a high-quality treated water product, it is associated with processes that help maintain cleaner, more environmentally friendly water systems.

This study examines the properties of Alpha Omega Water® using Fourier-transform infrared spectroscopy (FT-IR), proton nuclear magnetic resonance (NMR) spectroscopy, electrochemical impedance spectroscopy (EIS), and quantum chemical calculations based on Density Functional Theory (DFT). Treated water was compared with untreated control samples to evaluate possible differences in molecular organization and electrical behavior.

The results showed measurable differences in spectroscopic characteristics, impedance response, and modeled water-cluster parameters between treated and control samples under the applied experimental conditions.

These findings may be consistent with differences in the local hydrogen-bond environment and the associated physicochemical behavior of water.

These results indicate that Alpha Omega Water® possesses properties relevant to processes that improve the physicochemical characteristics of water, thereby contributing to the maintenance of a cleaner, more environmentally favorable water environment.

Keywords: Alpha Omega Water, hydrogen bonds, water clusters, FT-IR, NMR, DFT, EIS

INTRODUCTION

Water remains a subject of considerable scientific interest due to the complexity of its hydrogen-bond network and its influence on physicochemical behavior [1–4]. In recent years, increasing attention has been directed toward treatment methods that may alter water's structural and dynamic properties. The present study investigates the Alpha Omega Water® Crystal Instrument and its effect on water using a combination of experimental and theoretical approaches [5]. A comparative analysis was performed between treated water and control samples to evaluate possible differences in molecular organization and electrical response. The research integrates Fourier-transform infrared spectroscopy, nuclear magnetic resonance spectroscopy, and electrochemical impedance spectroscopy as complementary analytical methods [2,4–6]. In addition, Density Functional Theory calculations were applied to model water clusters and to examine their relative structural stability. This multidisciplinary methodology enables assessment of hydrogen-bond arrangements from both experimental and computational perspectives [2–6]. The results indicate that treated water exhibits measurable differences in spectroscopic characteristics, impedance behavior, and modeled cluster parameters relative to the control under the present experimental conditions.

These observations may be consistent with differences in the local hydrogen-bond environment and associated physicochemical responses of water, although the underlying molecular interpretation remains indirect and model-dependent [2–7]. Therefore, the study contributes to the discussion of water-related spectroscopic and electrochemical phenomena by combining spectroscopy, electrochemistry, and molecular modeling.

MATERIALS AND METHODS

Alpha Omega Water® 220011 Crystal Instrument

For water treatment, an Alpha Omega Water® 220011 Crystal Instrument, manufactured by SIA JL Ventures, AO Water Technologies (Kekavas Novads, LV-2111, Latvia), was used [5].

The manufacturer reports that the instrument includes components and construction materials compliant with relevant technical and drinking-water-related standards, including TÜV-tested elements and, where applicable, DVGW-certified piping components. Water treatment was performed by installing the Instrument within the municipal water supply network, using drinking water compliant with Directive (EU) 2020/2184 of 16 December 2020. The instrument contains



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water-conducted elements coated with gold and silver, and the standard acrylic housing is replaced with a synthetic quartz crystal housing of 99.99% purity.

The Alpha Omega Water 220011 Crystal Instrument has technical specifications for installation. The housing consists of a purely crystalline cylinder. The parameters are 65 cm in length, 8 cm in diameter, and 6.5 kg in weight. The instrument contains certified copper pipes and brass. Untreated tap water from the same supply line was used as the control. The experimental samples are referred to as “AO-treated water”, and both treated and control samples were stored under identical laboratory ambient conditions prior to analysis. Each analytical method was performed in five replicate measurements for both AO-treated and control samples.

NMR Spectroscopy and DFT Calculations of Water Clusters and Hydrogen Bonding

Nuclear magnetic resonance (NMR) spectra were recorded on a Bruker Avance II+ 600 MHz spectrometer (Billerica, MA, USA) equipped with a 5 mm direct detection dual broadband probe at 298 K [2]. Water samples were analyzed following established NMR procedures and the results were published in [5]. Theoretical calculations on small water clusters and hydrogen-bonding motifs were performed using Gaussian 16 [9]. Cluster geometries were optimized using a combination of quantum-chemical methods, including M06-2X/aug-cc-pVDZ, B3LYP/6-31++G, and MP2-based approaches [11–14]. NMR shielding tensors were computed using the GIAO approach [15]. The study was performed at the Institute of Organic Chemistry with Centre of Phytochemistry, Bulgarian Academy of Sciences.

Fourier-transform infrared (FT-IR) spectroscopy

The water samples were analyzed using Fourier-transform infrared (FT-IR) spectrometry [8]. The FT-IR spectra in our study were recorded with a “Thermo Nicolet Avatar 360 FT-IR” spectrometer (Waltham, MA, USA), equipped with a DTGS detector in the region 400–4000 cm^{-1} , accumulating 64 scans at a spectral resolution of 2 cm^{-1} . The experiments were performed at 298.15 K. All measurements were conducted at the Institute of General and Inorganic Chemistry, Bulgarian Academy of Sciences (BAS), Sofia, Bulgaria.

Electrochemical Impedance Spectroscopy (EIS)

The electrical and conductivity studies were conducted at temperatures close to 293.15 K using BioLogic potentiostat/galvanostat (SP-200), Claix,

France. Complex electrical impedance spectroscopy was applied in the 1 Hz–1000 kHz frequency range, as in our prior studies [8,16,17]. For the ionic conductivity and permittivity measurements, water was poured between two parallel, flat nickel plates, forming a parallel-plate capacitor with a 1 mm gap. The plates’ dimensions were 20 mm/12 mm.

RESULTS

Results with NMR and Quantum-chemical calculations

Quantum-chemical calculations were used to model the electronic structure of small water clusters and their hydrogen-bonding arrangements. These calculations were considered alongside the NMR data for a qualitative comparison of experimentally observed spectral features with theoretically modeled cluster motifs. The NMR results for Alpha Omega Water showed differences relative to the control sample, enabling a qualitative comparison of experimentally observed spectral features with theoretically modeled hydrogen-bonded water clusters.

Special attention has been given to the relationship between cluster size and hydrogen-bonding patterns in theoretical water cluster models, which serve as simplified representations of the local hydrogen-bond environment.

The results for Alpha Omega Water indicate a stabilized hydrogen-bond network of the clusters, which corresponds to an improvement in the physicochemical properties through the Alpha Omega Water Crystal Instrument [10].

Fig. 1 presents quantum-chemical data for Alpha Omega Water for various cluster types and their structural organization.

Levels of theory: Method A – Møller–Plesset second-order perturbation theory (MP2), a post-Hartree–Fock ab initio method: MP2/aug-cc-pVTZ; Method B – Density Functional Theory (DFT): M06-2X/aug-cc-pVDZ; Method C – Møller–Plesset second-order perturbation theory (MP2), a post-Hartree–Fock ab initio method: MP2/6-31G*.

Model of hydrogen bonds structured from different numbers of water molecules for Alpha Omega Water®

The modeling approach of Sykes and Levitt is adapted as a conceptual framework for exploring hydrogen-bond networks in Alpha Omega water clusters [18]. The modeled hydrogen-bond organization across multiple clusters was used to discuss possible differences in structural motifs. Fig. 2 shows the

dependence on the number of water molecules in clusters and the hydrogen bonds.

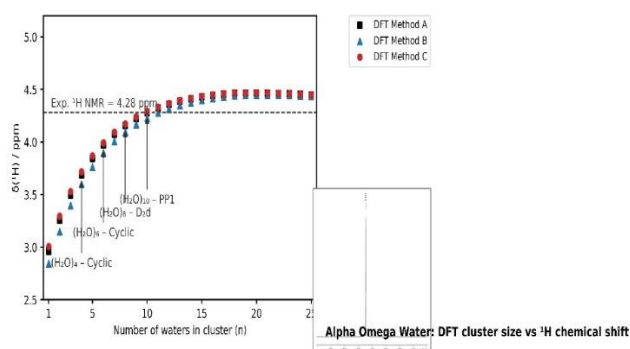


Fig. 1. Quantum chemical data for various types of clusters and their structural organization

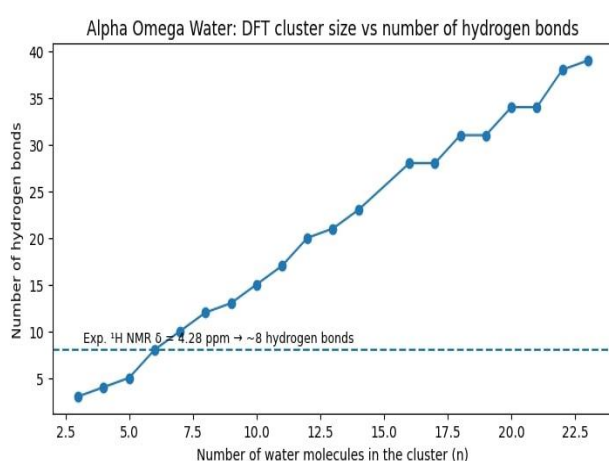


Fig. 2. Dependence on the number of water molecules in clusters and hydrogen bonds

The results show pronounced differences between the modeled configurations for Alpha Omega Water as a sample in hydrogen-bonded systems with $n = 2-39$ and cluster sizes of $n = 3-23$ water molecules, compared to a control sample. The results for Alpha Omega Water cover the entire investigated range of hydrogen bonds at the maximum number of water clusters described in the model. These results are expressed relative to tap water, in which the number of water molecules in clusters and hydrogen bonds is lower.

Electrochemical Impedance Spectroscopy (EIS) for Alpha Omega Water®

Electrochemical impedance spectroscopy (EIS) was employed to characterize the electrical and dielectric response of Alpha Omega Water samples and untreated tap-water control samples [8,16,17]. Measurements were conducted using a BioLogic

potentiostat/galvanostat (SP-200, Claix, France) under controlled temperature conditions. The complex impedance spectra were recorded over the selected frequency range using established methodologies for liquid electrolyte systems.

For the measurements, 100 μL of each water sample was placed between two parallel flat nickel electrodes, forming a plane-parallel capacitor. The electrode separation was 0.6 mm, and the electrode dimensions were 13 mm $\times$ 14.5 mm. A sinusoidal alternating voltage with an amplitude of 10 mV was applied.

The complex electrical impedance

$$Z^* = Z' + iZ''$$

was measured as a function of the applied frequency, providing simultaneous access to the real (Z') and imaginary (Z'') components of the impedance response.

Electrochemical impedance spectroscopy (EIS) is a widely used and well-established technique for investigating conductivity, capacitance, and diffusion-related processes in electrolyte and liquid systems. In aqueous media, EIS provides information on frequency-dependent charge transport, interfacial polarization, and dielectric relaxation phenomena.

Ionic composition, molecular mobility, dissolved species, electrode polarization effects, and the dynamic organization of hydrogen bonds influence the electrical behavior of water. These factors collectively determine the system's dielectric response when subjected to an alternating electric field. The dielectric properties of water can be described using the complex dielectric permittivity:

$$\varepsilon^* = \varepsilon' - j\varepsilon''$$

where ε' is the real part of the dielectric permittivity (dielectric constant), and ε'' represents dielectric losses associated with relaxation and conductive processes.

The real and imaginary parts of the complex impedance can be used to estimate ε' and ε'' through established relationships:

$$\begin{aligned} (1) \quad \varepsilon'(f) &= \frac{Z''}{((Z')^2 + (Z'')^2)\omega C_0} \\ (2) \quad \varepsilon''(f) &= \frac{Z'}{((Z')^2 + (Z'')^2)\omega C_0} \end{aligned}$$

where C_0 is the vacuum capacitance defined as $C_0 = \varepsilon''A/t$, ε'' is the permittivity of free space (8.85×10^{-12} F/m), A is the electrode area, and t is the electrode separation. The angular frequency is given

by $\omega = 2\pi f$. These relationships are approximations valid under the assumptions of a uniform electric field and a stable electrode geometry.

In the investigated frequency range, the impedance spectra of the water samples exhibit regions of approximately linear behavior in Nyquist representation (Z'' vs. Z'). Such linear sections are commonly associated with diffusion-capacitive impedance responses in liquid electrolyte systems.

The linear portions of the impedance curves were approximated using the relation:

$$Z'' \approx mZ' + b \quad (3)$$

where m is the slope of the linear fit, reflecting the phase relationship between the real and imaginary components of the impedance, and b is the intercept with the imaginary impedance axis.

The quality of the linear approximation was evaluated using standard statistical parameters, including the coefficient of determination (R^2) and the residual sum of squares (RSS). These parameters quantify the degree of agreement between the experimental data and the applied linear model. Nyquist complex impedance plots were obtained for the investigated water samples and compared with a reference water sample measured under identical experimental conditions. Differences in slope, intercept, and degree of linearity were observed among the samples.

Fig. 3 illustrates the EIS results of Alpha Omega Water (green and red curves) and the control sample with tap water (black curves).

The extracted parameters (R^2 , RSS) are summarized in Table 1. Variations in these parameters indicate differences in the electrochemical impedance response of the samples, which may arise from differences in ionic transport, polarization effects, electrode-interface phenomena, and relaxation dynamics within the aqueous medium.

The impedance response of water reflects the combined contribution of ionic conductivity, dielectric polarization, and frequency-dependent relaxation processes. A higher degree of linearity in the Nyquist representation, together with low residual errors, indicates a reproducible and well-defined electrochemical impedance response within the analyzed frequency range.

Several studies have proposed that transient molecular associations and hydrogen-bonded configurations in water may influence its electrical and dielectric behavior. Such models provide theoretical frameworks for interpreting experimental

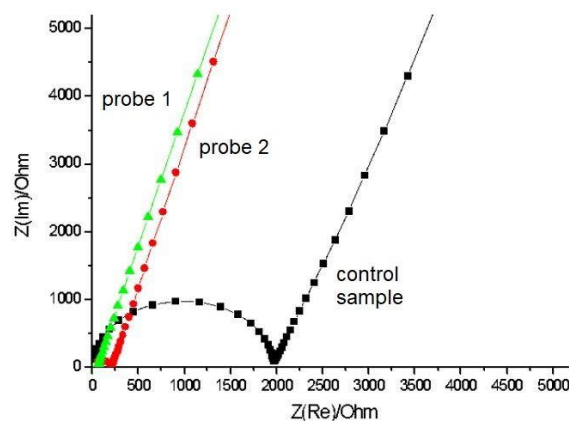


Fig. 3. EIS results of Alpha Omega Water (green and red curves) and the control sample with tap water (black curves)

Table 1. R^2 and RSS results of Alpha Omega Water

Type of sample	R^2	RSS
Sample 1 Alpha Omega Water	0.985627	8.7433
Sample 2 Alpha Omega Water	0.981516	8.6173
Control Sample Tap Water	0.977215	11.93

observations. However, interpretation of impedance data in terms of molecular organization remains indirect and strongly model-dependent. Such models provide theoretical frameworks for interpreting experimental observations. Consequently, any interpretation of impedance data in terms of molecular organization should be regarded as indirect and model-dependent.

Electrochemical impedance spectroscopy is a sensitive and reproducible method for characterizing the frequency-dependent electrical and dielectric response of water. The analysis of complex impedance spectra, combined with linear approximation and statistical evaluation, enables a comparative assessment of different water samples under controlled conditions.

The applied methodology provides comparative information on ionic transport and polarization behavior among the samples. This approach is suitable for controlled comparative studies of water samples using electrochemical impedance techniques.

Sample 1 and Sample 2 of Alpha Omega Water exhibit nearly linear impedance responses ($R^2 = 0.985627$ and 0.981516 , respectively) with low residual errors ($RSS = 8.7433$ and 8.6173). The control sample with tap water shows lower linearity ($R^2 = 0.977215$) and a higher residual sum of squares ($RSS = 11.92$), indicating greater residual errors.

In Fig. 3, the differences between Alpha Omega Water and the control sample are clearly expressed. These differences indicate pronounced variations, demonstrating that Alpha Omega Water exhibits a stronger impedance response than the control sample. This reflects more pronounced processes associated with ionic mobility, dielectric polarization, interfacial charge distribution, and water relaxation dynamics.

Molecular Modeling with the Results of Fourier Transform Infrared Spectroscopy (FT-IR)

FT-IR records how water absorbs infrared light, which depends on the vibrations of water molecules and the hydrogen bonds between them. When these data are combined with molecular modeling, vibrational analyses are performed. This allows the assessment of vibrational features that may be consistent with specific hydrogen-bonding environments or hydration motifs [2,10].

Fig. 4 demonstrates the FT-IR spectrum of Alpha Omega Water®

The peaks and the regions in the infrared (FT-IR) spectrum of Alpha Omega Water are more pronounced than those of the control sample, which is not with expressed peaks. The individual peaks indicate the following:

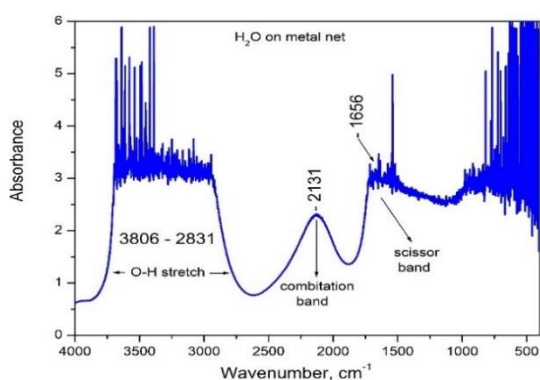


Fig. 4. FT-IR spectrum of Alpha Omega Water®

Region 3800–2830 cm^{-1} : O–H vibrations

This is the most characteristic region of water. The broad band arises from stretching vibrations of the O–H bonds. The width and shape of this band

are consistent with hydrogen bonding in liquid water. Different local environments, including more weakly and more strongly hydrogen-bonded O–H groups, may contribute to the band profile. This region is sensitive to the hydrogen-bond network. Different local environments (free and hydrogen-bonded O–H groups) are observed. This region indicates a more structured hydrogen-bond network in Alpha Omega water compared to the control sample.

Around 2131 cm^{-1} : Combination band

The combination band arises from a combination of stretching and bending modes that are sensitive to collective molecular motions. For Alpha Omega Water, this band is pronounced and is consistent with intermolecular interactions characteristic of liquid water according to the control sample.

Around 1656 cm^{-1} : H–O–H bending (scissoring) mode

This band is associated with deformation vibrations of the H–O–H angle and is sensitive to hydrogen bonding and local molecular environment. In the present study, differences relative to the tap-water control may reflect differences in local hydrogen-bonding conditions, although the interpretation is not unique. For Alpha Omega Water, this indicates more pronounced hydrogen-bond dynamics compared to the control sample with tap water.

Low-frequency region ($<1000 \text{ cm}^{-1}$)

For Alpha Omega Water, the low-frequency region ($<1000 \text{ cm}^{-1}$) may include contributions from librational motions and collective vibrations of the hydrogen-bond network. The differences compared to the tap-water control reflect changes in the measured vibrational response, with enhanced cooperative molecular ordering observed in Alpha Omega Water.

Overall, the spectral profile of Alpha Omega Water shows more pronounced and well-defined vibrational features across the investigated peaks than the control sample. The observed differences in the combination band around 2131 cm^{-1} , the H–O–H bending mode around 1656 cm^{-1} , and the low-frequency region below 1000 cm^{-1} consistently indicate altered intermolecular interactions, enhanced hydrogen-bond dynamics, and stronger cooperative organization of the water structure. Compared with the control sample, Alpha Omega Water exhibits a more distinct and intensified vibrational response, suggesting a more ordered hydrogen-bond network and altered molecular dynamics.

CONCLUSIONS

Alpha Omega Water® exhibited measurable differences in selected spectroscopic, electrochemical, and quantum-chemical parameters compared with the untreated control water under the applied experimental conditions.

The FT-IR results revealed differences in vibrational features associated with hydrogen bonding. The EIS measurements showed differences in impedance behavior associated with changes in ionic transport and polarization response. The quantum-chemical calculations on small water clusters also showed differences in relative cluster stability and hydrogen-bond arrangements.

Taken together, the results indicate that treatment with the Alpha Omega Water® is associated with measurable physicochemical differences in water under controlled laboratory conditions. These findings also suggest that Alpha Omega Water® possesses properties relevant to processes that improve the physicochemical characteristics of water, thereby contributing to the maintenance of a cleaner, more environmentally favorable water environment.

From an ecological perspective, these findings demonstrate that Alpha Omega Water® is relevant to environmental sustainability through its association with improved water quality and a cleaner, more favorable water environment.

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