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COMPARATIVE STUDY ON STRUCTURE AND PROPERTIES OF WATER BY INFRA RED AND OPTO-MAGNETIC SPECTROSCOPY

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Abstract. Water is perhaps the most studied material today; it has been studied with different tools and methods, but its behavior and function remain elusive. Using water-light interaction based methods we wanted to analyze the connection between the structure of water and the effect this water has.

The methods used for research of several spring waters, commercial mineral waters and tap waters are - IR spectroscopy with novel Aquaphotomics approach and Opto-magnetic spectroscopy. Using these methods, it was shown that under just slightly different conditions (atmospheric pressure, temperature, and humidity) not just that different waters behave differently, but the same water shows different behavior. This behavior which comes as a result of rich water dynamics which is a response to changes in its surroundings was captured and described using aquagrams and opto-magnetic fingerprint spectra.

Keywords: drinking water, water quality, opto-magnetic spectroscopy, near infra red spectroscopy, aquaphotomics.

1. INTRODUCTION

Water is perhaps the most studied material today; it has been studied with different tools and methods, but its behavior is still the subject of intensive scientific research. At a molecular level, water is not a homogeneous structure, but rather dynamic equilibrium among changing percentages of assemblages of different oligomers and polymer species. The structure and these assemblages or units themselves are dependent on temperature, pressure and composition [1].

Using water-light interaction based methods we wanted to 'shed some light' on the water structure in a hope to see 'inside the water' and if it is possible to find some conclusions how different molecular structure of water gives different properties.

We investigated several spring waters, commercial mineral waters and tap waters by the means of light-matter interaction methods - IR spectroscopy with novel Aquaphotomics approach [2] and Opto-magnetic spectroscopy [3, 4]. Using these methods, it was shown that under just slightly different conditions (atmospheric pressure, temperature, and humidity) not just that different waters behave differently, but the same water shows different behavior. This behavior which comes as a result of rich water dynamics - constant structuring and restructuring, as a response to change in its surroundings, was captured and described using aquagrams and opto-magnetic fingerprint spectra.

2. MATERIAL

The samples investigated were Millipore pure water (Milli Systems Co., USA), two kinds of commercial natural mineral waters from Serbia (Aqua Viva, Knjaz Milos - carbonated), two kinds of tap water from Serbian cities of Belgrade (Belgrade tap water) and Zrenjanin (Zrenjanin tap water), four kinds of natural spring waters from Japan (Silver, Gold, Kongou, and Copper which is a mixture of Silver and Kongou water) and an Austrian mineral water Grander Blue water. Only Knjaz Milos water was carbonated.

Commercial mineral waters were obtained at a supermarket, and the samples of tap waters were collected using polyetilen bottles rinsed thoroughly with pure water prior to collecting.

All mineral water brands and spring waters were in original plastic bottles with plastic screw caps except Grander Blue water brand which was in a glass bottle with a metal screw cap. The bottled water capacity of the samples ranged between 0.5 and 1.5l. After the collection of samples, they were

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brought to the laboratory, where they were stored in their original bottles at room temperature and in dark until analysis.

Manufacturer labels on the bottles were used as a source of basic information about particular water sample, as well as the data from the manufacturers' websites [5,6]. Physico-chemical properties of tap waters were obtained from the ref [7,8]. These data are summarized in Table 1.

3. METHOD

3.1. Near-infrared spectral analysis and Aquaphotomics

NIR transmission spectra of water samples in the 400-2500nm region were recorded using NIR Systems 6500 spectrophotometer (FOSS-NIRSystems). A quartz liquid sample cell was used as a container. Order of taking spectra for water samples was random, and for each water sample 3 consecutive spectra were recorded.

The experiment was conducted 2 times, and each time the ambient conditions were recorded. These recorded data are presented in Table 2.

Only the region of the first overtone of water was used in analysis (Fig.1) and for two experiments in total 120 spectra was recorded.

For each experiment, the spectra were normalized, pure water spectra subtracted and aquagrams are developed in accordance with Aquaphotomics approach [2].

3.2. Opto-magnetic spectroscopy

Opto-magnetic fingerprint method, or also called Opto-magnetic convolution spectroscopy is a novel method based on light-matter interaction (for more detailed description of the method see references [3, 4, 9]).

Table 1. Physico-chemical properties of investigated waters

WATERS				As	B	Ca	Fe	K	Mg	Na	HCO_3^-	Cl^-	SO_4^{2-}
Country	Water	pH	EC [µS/cm]	mg/L									
Serbia	Zrenjanin	7.56	928	71.9	895	27.4	87.5	1.2	13.6	275	846	17.4	0.97
	Beograd	7.56	318	0.29	22.2	61.1	2.34	1.1	11.1	6.5	194	11.3	37.5
	Aqua Viva	7.62	504	0.0006	0.1	90.1	0.05	2.1	13.3	13.7	341	20.6	28.1
	Knjaz Milos	5.7	*	0.0006	*	108.2	0.05	16.6	53.5	229.5	1281	10.7	13
Japan	Copper	6.59	171	*	*	11.6	*	*	4.49	18.8	*	4.703	1.898
	Silver	6.6	1700	*	*	180	*	*	57.8	165	*	212.578	0.248
	Gold	6.18	357	*	*	29.5	*	*	7.69	37.6	*	24.164	0.014
	Kongou	No available data											
Austria	Grander Blue Water			*	*	42	*	*	25	3.8	*	0.9	58.1

Table 2. Experiments ambient condition

Experiment No.	**Date**	**Temperature [°C]**	**Pressure [hPa]**	**Humidity [%]**
1	3/10/2011	23.8	1003.7	13
2	3/16/2011	24.4	992.8	14

The device used for taking digital images is comprised of a digital camera (Canon XS 105, Cannon Inc) in a specially designed housing with an additionally placed two LED systems (six light emitting diodes per system) arranged in a circle in front of an objective for illuminating surface of a sample. First LED system illuminates sample by providing incident white diffuse light under angle of 90°. The second LED system provides incident white diffuse light under angle of 53° - the angle under which light reflected from the water surface will be completely polarized (Brewster angle for water [3]).

Since reflected polarized light contains only electrical component of light-matter interaction, the difference between reflected white light (electromagnetic nature) and reflected polarized white light can serve as a measure of magnetic properties of matter. To know magnetic properties of matter is to better understand quantum nature of matter.

For each water, at least 10 pairs of white and polarized digital images were taken. The images used are in RGB system of colors, and only color data from red and blue color channel were used for both white diffuse light (W) and reflected polarized white light (P). Algorithm for data analysis is based on chromaticity diagram called Maxwell' triangle and spectral convolution operation according to ratio (R-B) & (W-P). The abbreviated designation means that Red minus Blue wavelength of white light and reflected polarized light are used in spectral convolution algorithm to calculate data for opto-magnetic fingerprint of matter. Using this algorithm for spectral convolution, 10 pairs of white and polarized images of water sample, give 10 spectra per water sample.

Detailed experiment arrangement sketch and scheme of developing spectra based on digital images, is given in Fig. 2.

In total for 2 experiments 200 opto-magnetic spectra was obtained.

4. RESULTS AND DISCUSSION

Using water-light interaction based methods : infra red and opto –magnetic spectroscopy 10 different types of water were analyzed, some of which were reported to have remarkable properties. Aquagrams in a simplified fashion present 12 characteristic wavelength ranges in the area of the 1st overtone of water in NIR spectra, repeatedly found to be of great importance for functioning of biological systems.Opto-magnetic spectra give another type of insight into the water organization and dynamics, by presenting paramagnetic and diamagnetic properties of water which are related to its constant structuring and restructuring (making and breaking of water clusters).

Results are presented in a form of aquagrams and opto-magnetic fingerprint spectra of each kind of water (Figures 3-12). For two separate experiments performed, these two types of diagrams were qualitatively analyzed and compared. As it can be seen from the opto-magnetic spectra , pure water (Fig. 3)shows stable para/diamagnetic behavior in both experiments Pure water results from analysis of NIR spectra are represented with a zero line on the aquagrams (subtraction technique).

For opto-magnetic spectra, main spectral characteristics described in Fig. 2, were extracted and summarized in Table3.

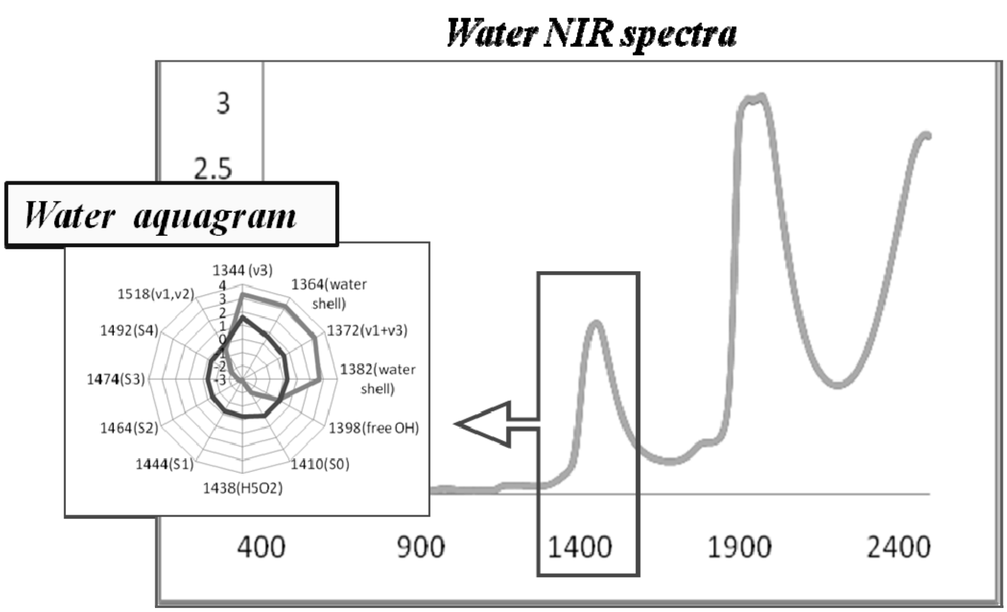


Figure 1. The region of first overtone of water where 12 most important wavelength ranges (WAMACs – Water matrix Coordinates) are found to be with respect to living systems functioning [2]. These 12 wavelength ranges are used for graphical representation in a form of aquagrams

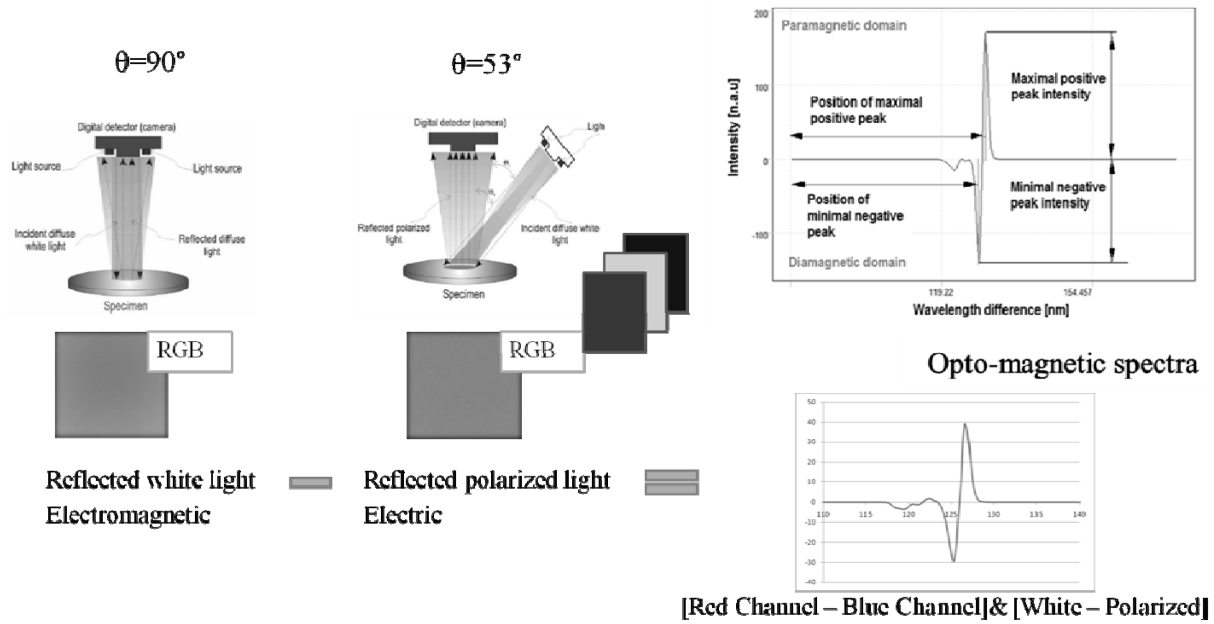


Figure 2. Opto-magnetic spectroscopy : The experimental arrangement sketch showing relative positions of light sources for white and reflected polarized light (left); Scheme of developing spectra based on digital images (reflected light) and most important characteristics of opto-magnetic fingerprint spectrum (edited from ref. [5])

Table 3. Main spectral characteristic of opto-magnetic fingerprint spectra of analyzed waters

Exp. No.	Water	Positive peaks		Negative peaks	
		Intensity	Wavelength difference [nm]	Intensity	Wavelentgh difference [nm]
1st .	Pure water	39.076	126.558	-29.684	125.26
	Aqua Viva	40.172	127.109	-30.736	125.497
	Grander Blue water	34.383	127.606	-24.455	126.106
	Copper water	31.433	127.606	-25.696	126.106
	Silver water	32.928	127.606	-26.357	126.106
	Belgrade tap water	34.674	127.329	-25.954	125.73
	Knjaz Milos	7.621	129.073	-3.493	125.26
	Zrenjanin tap water	40.103	129.073	-37.209	126.558
	Gold water	29.106	127.606	-20.958	126.106
	Kongou water	28.439	127.886	-23.250	126.323
2nd	Pure water	33.527	126.779	-22.331	125.26
	Aqua Viva	33.662	127.109	-22.761	125.497
	Grander Blue water	28.858	128.104	-18.330	126.558
	Copper water	32.783	127.606	-21.340	126.106
	Silver water	35.814	127.109	-23.287	125.497
	Belgrade tap water	30.976	126.779	-21.469	125.26
	Knjaz Milos	30.571	127.109	-20.723	125.26
	Zrenjanin tap water	51.728	126.558	-46.112	124.981
	Gold water	37.652	127.109	-24.762	125.497
	Kongou water	31.442	127.606	-23.587	126.106

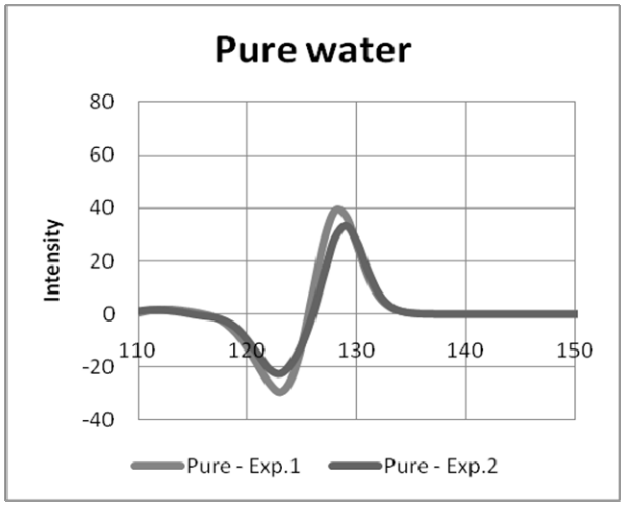
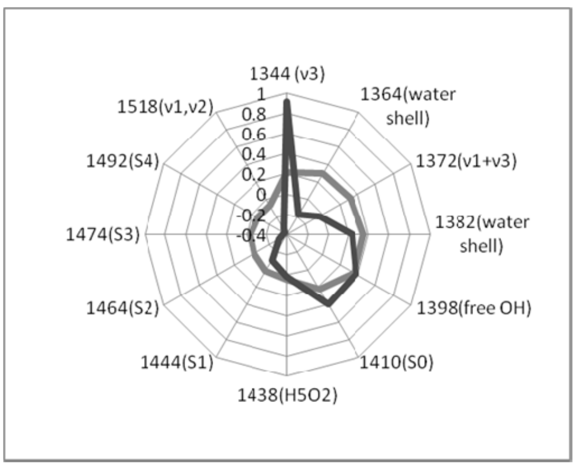


Figure 3. Opto-magnetic spectra of Pure water



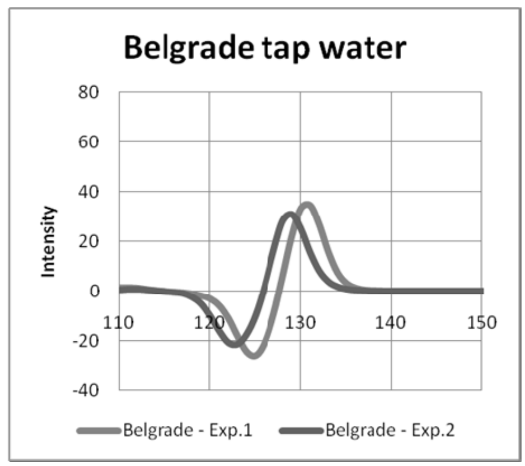
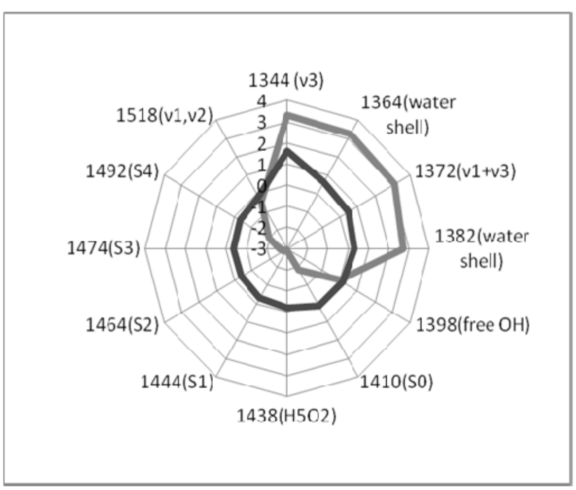


Figure 4. Aquagram and Opto-magnetic spectra of Belgrade tap water



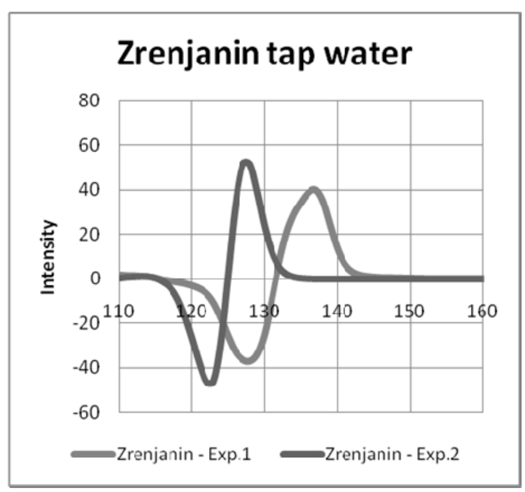


Figure 5. Aquagram and Opto-magnetic spectra of Zrenjanin tap water

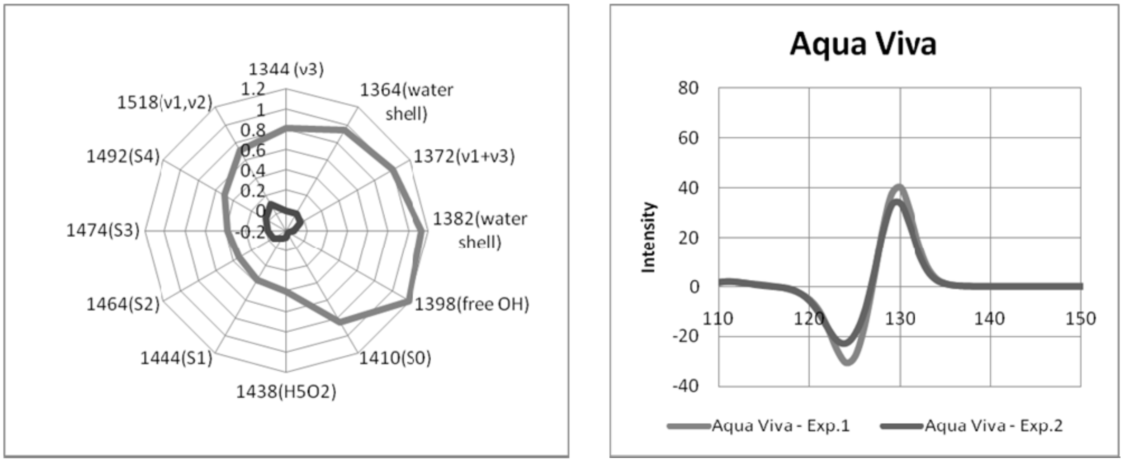


Figure 6. Aquagram and Opto-magnetic spectra of commercial mineral water from Serbia – Aqua Viva

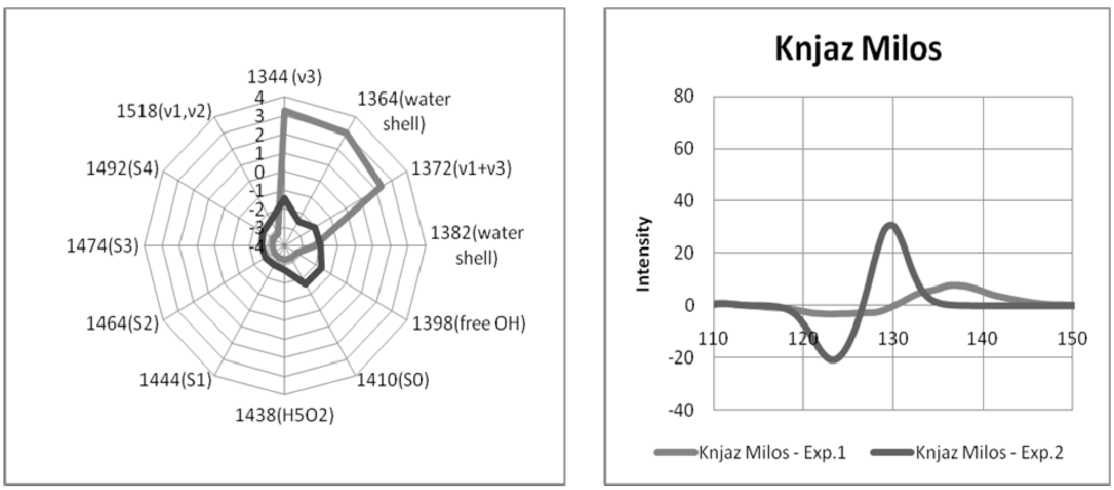


Figure 7. Aquagram and Opto-magnetic spectra of commercial mineral water from Serbia – Knjaz Milos

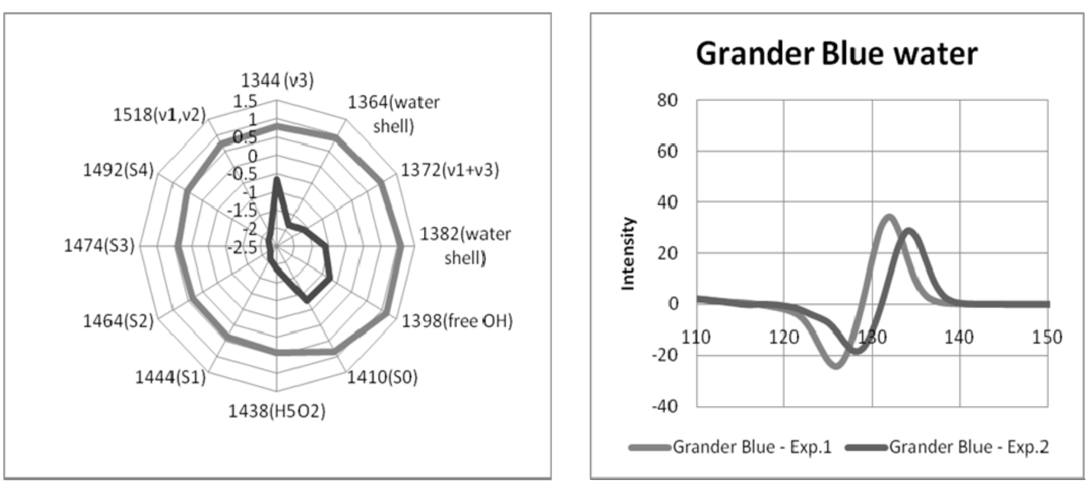


Figure 8. Aquagram and Opto-magnetic spectra of mineral water from Austria – Grander Blue water

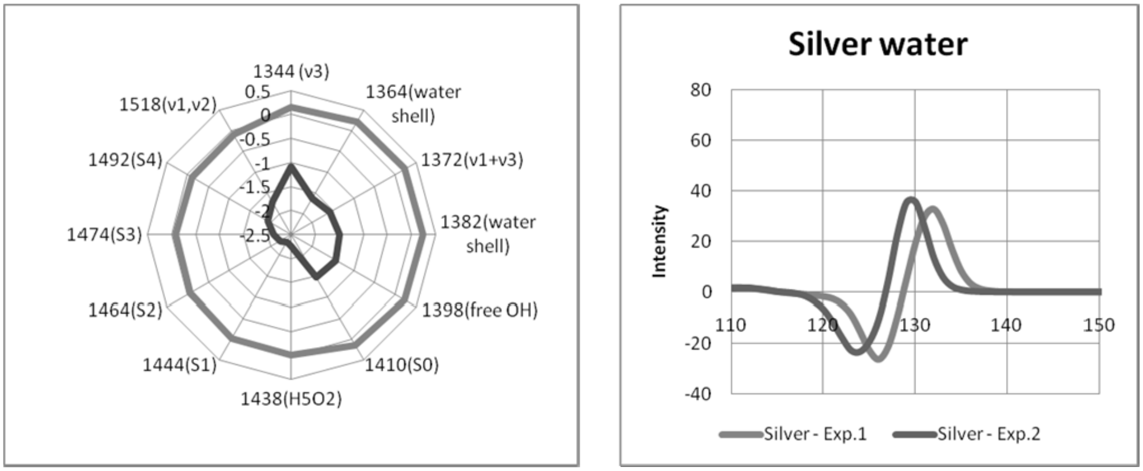


Figure 9. Aquagram and Opto-magnetic spectra of spring water from Japan – Silver water

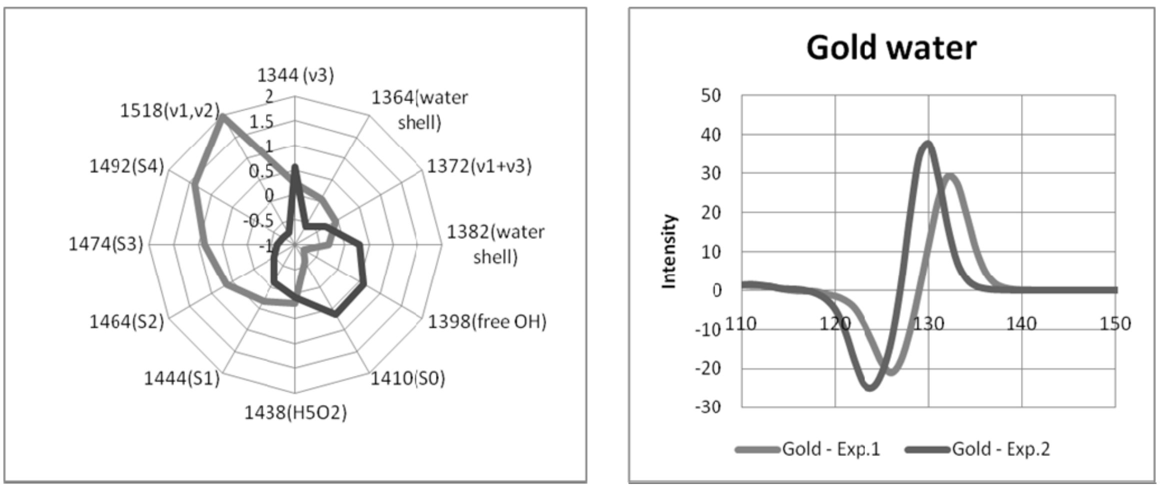


Figure 10. Aquagram and Opto-magnetic spectra of spring water from Japan – Silver water

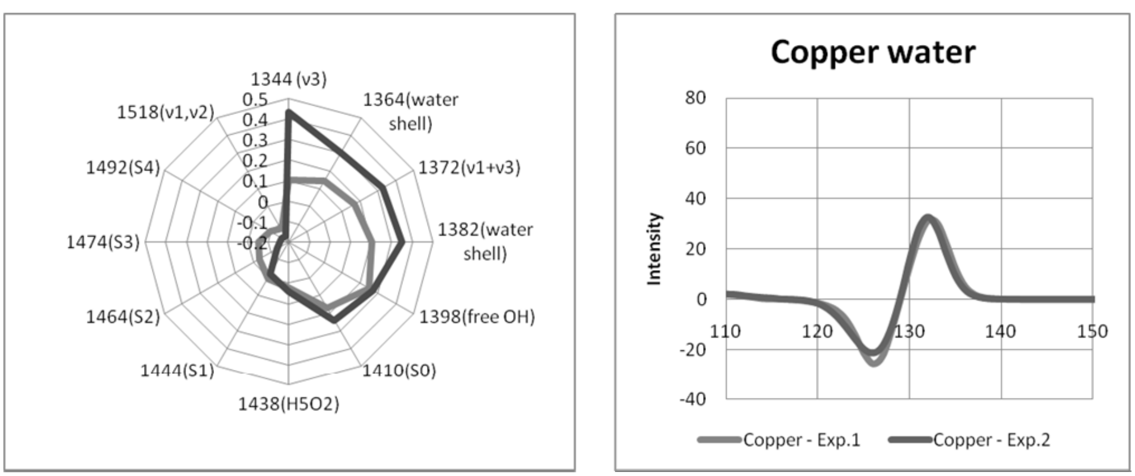


Figure 11. Aquagram and Opto-magnetic spectra of mixed water from Japan – Copper water

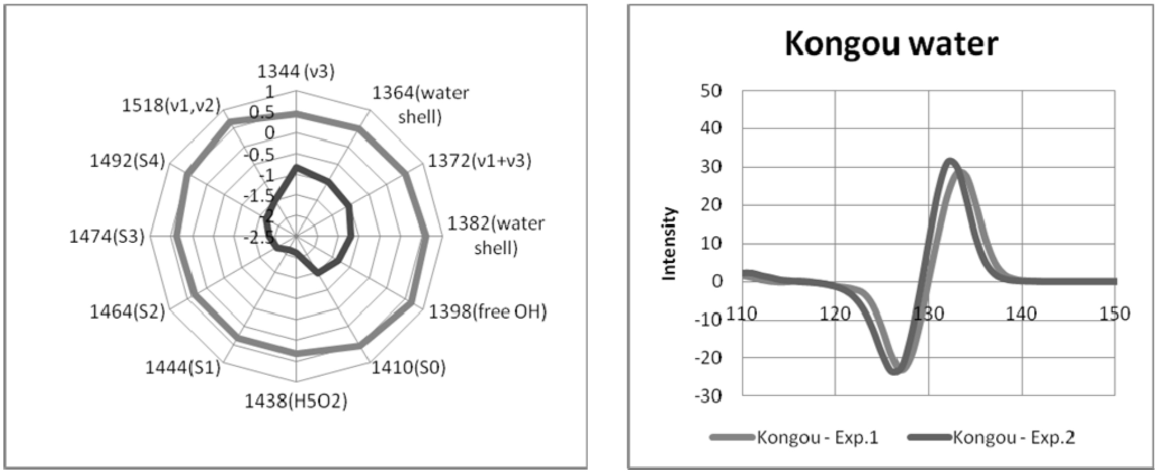


Figure 12. Aquagram and Opto-magnetic spectra of spring water from Japan – Kongou water

5. CONCLUSION

In this study several types of water: tap waters, commercial mineral waters and spring waters originated from different countries were analyzed using NIR and OM spectroscopy. Both methods, NIRS coupled with Aquaphotomics approach and Opto-magnetic spectroscopy have been proved to be valuable tools for non-invasive dynamic analysis of biological and aqueous systems.

Using these methods , it was shown that under just slightly different conditions (atmospheric pressure, temperature, and humidity) not just that different waters behave differently, but the same water shows different behavior, which may be result of its micro and macro heterogeneity, evaporation and response to external environment. Largest differences of the opto-magnetic spectra can be observed in the case of Zrenjanin tap water and Knjaz Milos water, but in the case of the Knjaz Milos this difference is a result of decarbonation.

Strongest paramagnetic and diamagnetic properties are attributed to Zrenjanin tap water. It also has highest ratio of para/diamagnetic intensities. Large intensities of para/diamagnetism can be seen in Gold water also, but as it can be seen from respective aquagrams different water molecular conformations are present. It is interesting fact that out of all analyzed waters, only this water is reported to be toxic [8].

Most stable opto-magnetic spectra are found in the case of Aqua Viva, Kongou and Copper water, all of which reported to have beneficial health effects.

With further insights into the structure of water, comparative studies such as this, which are focused on different aspects of water, could be proven to be invaluable in assessing water quality and how particular water could affect living systems.

6. ACKNOWLEDGMENTS

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КОМПАРАТИВНА СТУДИЈА СТРУКТУРЕ И СВОЈСТАВА ВОДЕ ПРИМЕНОМ ИНФРАЦРВЕНЕ И ОПТО-МАГНЕТНЕ СПЕКТРОСКОПИЈЕ

Сажетак. Вода је један он највише проучаваних материјала данас при чему се користе различите методе и технике, али понашање воде и њена функција остају нејасни. Уз помоћ две методе засноване на интеракцији светлости и материје, урађена је компаративна анализа воде у нади да ће то омогућити увид у структуру воде и како се она може повезати са ефектима које вода испољава.

Испитивано је неколико изворских вода, као и комерцијалних минералних вода и вода из градских водовода, а методе коришћене за испитивање су инфрацрвена спектроскопија – у комбинацији са новим аквафотомика приступом и опто-магнетна спектроскопија. Коришћењем ових метода установљено је да свака вода показује другачије понашање, као и да једна иста вода показује варијације у понашању као реакцију на измењене спољне услове (атмосферски притисак, температура, влажност ваздуха). За графички приказ ових промена, које настају као резултат изразите динамичности воде, коришћени су акваграми и опто-магнетни фингерпринт спектри.

Кључне речи: вода за пиће, квалитет воде, опто-магнетна спектроскопија, блиска инфра црвена спектроскопија, аквафотомика.