

What is the type of water that you use?

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Introduction

In agricultural materials absorbed water preferentially occupies locations where it can form hydrogen bonds. The vibrations of bonds involving hydrogen have harmonics and combination bands with appreciable absorbance in the near infrared (NIR) region of the spectrum.

The NIR region is particularly useful in studying the absorptions of bonds containing hydrogen.¹ The strongest NIR absorption for water, the $\nu_2 + \nu_3$ combination band of the asymmetric stretch (ν_2) and the bending vibration (ν_3), is at about 1923 nm. The first overtone of the symmetric stretch (ν_1), at about 1400 nm, is significantly weaker than the $\nu_2 + \nu_3$ combination band, but can usually be discerned.

The amount of moisture absorbed by materials is important in many areas of technology because of the influence of moisture on mechanical properties, electrical properties, adhesion, corrosion, hydrolysis reactions, spectral characteristics, and functionality in general. Measurements of absorbance in the NIR region can be useful, not only for deducing the concentration of water but also for providing information about the nature of hydrogen bonding of the water to its surroundings.²

Water is not completely hydrogen bonded and the bonding decreases with increasing temperature.³⁻⁴ Goldstein and Penner⁴ assigned 1916 nm, 1953 nm, and 2000 nm to the peak positions of the NIR absorbances for water molecules in liquid water involved in 0, 1, and 2 hydrogen bonds, respectively.

Most non-polar ('hydrophobic' or weakly 'hydrophilic') solutes do not dissolve in water beyond a very low limit. Even oxygen at atmospheric pressure produces only a low equilibrium concentration in water. Sometimes, instead of totally rejecting such solutes, water forms "cages" around each molecule to give clathrate compounds.⁵

The state of water in food products has been investigated by a large number of research units.⁶ In spite of employing advanced research methods and modern technological equipment, our knowledge on the subject is still incomplete.⁷ From time to time we learn about new original developments and new details supplementing earlier works on water behaviour in food.⁸⁻⁹

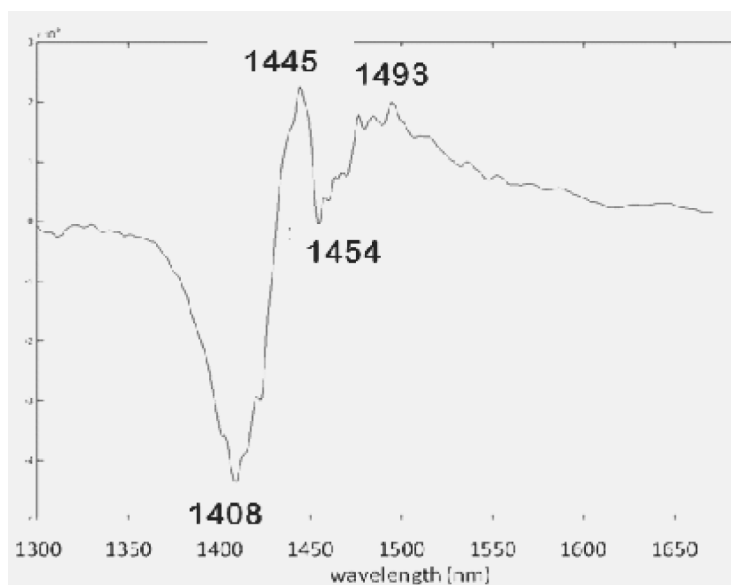


Figure 1. Spectrum of differences among Tap water samples.

Materials and methods

Several samples of different types of tap-water, collected from eight regional sources (Tap), and de-mineralised water samples (five samples) that had been demineralised by different pre-treatments, such as reverse osmosis (RO), de-ionisation (DI), bi-distillation (BD) were analysed. NIR spectra were recorded at 38°C by a NIRFlex N500 (BUCHI Italia, Assago, Milan) instrument in transmittance mode (pathlength 1 mm; quartz cuvettes) in the NIR range from 1300 nm to 1700 nm. (32 scan, resolution 4 cm⁻¹, 3 scans for each sample). The first derivative (SG 35, 2) and EMSC (2nd order) were applied as spectra pre-treatments. Data were processed by Unscrambler software v. 9.2 (Camo Inc., OSLO, Norway). Differences between replicate scans, and among different types of water were computed and statistically evaluated by applying the following equation: $[\sum_{(m,j)} \sum_{(n,i)} (\bar{A}_i - A_{ij})^2]^{1/2} / (m+n-1)$; where: m=number of spectra, n=number of data points, A=absorbance.

The conductivity (μS) was also tested on all samples by using a Metrohm 660 (Herisau, Switzerland) conductometer.

Samples were named in the following order: 1 = BD1; 2 = DI1; 3 = RO1; 4 = Tap1; 5 = BD2; 6 = DI2; 7 = Tap2; 8 = Tap3; 9 = Tap4; 10 = Tap5; 11 = Tap6; 12 = Tap7; 13 = Tap8.

Results and discussion

Variations in the absorption patterns among the water samples were detected. The main water absorption bands detectable in the NIR range from 1400 to 1550 nm showed changes in intensity

Table 1. Absorbance variability calculated on pre-treated spectra intra-replicates.

Samples	Differences among replicates
5	0.0000012
1	0.0000047
2	0.0000046
6	0.0000029
3	0.0000066
9	0.0000162
8	0.0000028
7	0.0000164
10	0.0000094
12	0.0000029
4	0.0000060
13	0.0000201
11	0.0000070

and position as a function of both the origin of water samples and the pre-treatment applied for their purification. The variability found among tap water samples highlighted specific wave-lengths where differences arose, as shown in Figure 1 for tap water samples.

Table 1 shows the variability in absorbance, calculated on pre-treated spectra, among replicate scans of the same sample.

Applying the same equation to calculate the variability on pre-treated spectra among different samples or grouped samples, the following data were found of absorbance differences among: a) Tap water samples: 2.07×10^{-5} ; b) BD samples: 5.65×10^{-6} ; c) BI samples: 5.19×10^{-6} ; d) pre-treated water samples: 9.16×10^{-6} . In all cases, higher variability was found between different samples than between replicates of the same samples.

The location of tap-water source (origin) seemed to have a strong influence on the spectral data. Conductibility values for these samples were highly correlated with their mineral concentration, probably due to the nature of soil from where the tap-water samples were collected. In particular, the conductivity values for all samples, expressed as μS , were respectively: 1 = 4.22; 2 = 5.53; 3 = 6.50; 4 = 7.99; 5 = 2.74; 6 = 5.75; 7 = 6.35; 8 = 5.38; 9 = 2.88; 10 = 6.65; 11 = 8.32; 12 = 7.31; 13 = 8.30.

Although most minerals have no absorbers in the NIR range, in this work a certain influence of conductance values on NIR water absorption bands was found. Figure 2 reports the conductivity vs mean absorbance values at 1408 nm for the group of samples named “tap water”.

These findings support the thesis that not only the mineral concentration, but also the types of minerals and their hydration capacities can affect water spectral response in the NIR range.

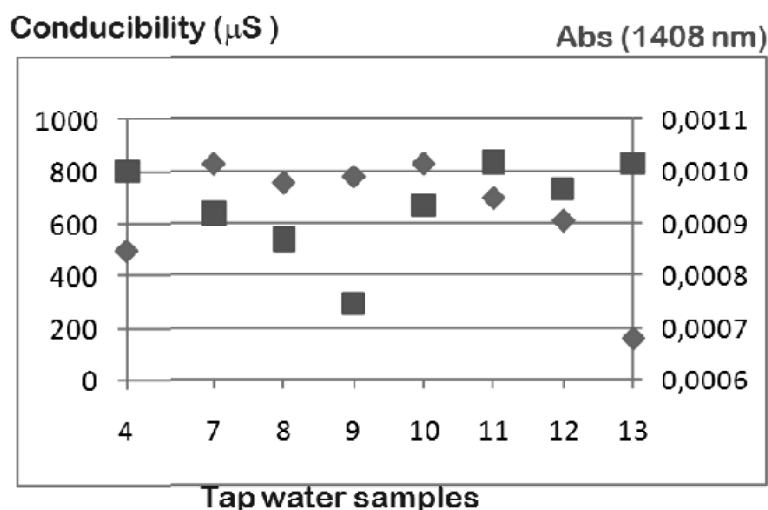


Figure 2. Plot of conductivity (■) vs mean absorbance values at 1408 nm for the Tap water samples.

Conclusions

These observations alert researchers in the NIR field to consider the contributions of the actual water spectral absorptions in their experiments, when water is used as solvent. Not only temperature can affect the NIR water spectrum, but also the origin and purity of the water. When working with any type of NIR applications involving aqueous solutions the type of the water should be indicated, including source, de-mineralisation pre-treatment used, and the corresponding μS value. Ideally such experiments should be repeated, using the same type of water.

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