Unveiling Water Clusters: Exploring Formation with Alternating Electric Fields

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Background

Water, which is essential to biological systems, has a complex network of hydrogen bonds that give it its unique behavior. This work investigates the formation of water clusters by microwaves in the MHz-GHz frequency range, with particular attention to their dynamic and structural characteristics. We explore how particular microwave frequencies promote cluster formation and stability, potentially impacting DNA and protein manipulation and other biological processes, using cutting-edge methods such as Raman spectroscopy. Our research offers fresh perspectives on the behavior of water in alternating electromagnetic fields, which has important ramifications for molecular biology, materials science, and biomedical engineering. This work could lay the groundwork for novel approaches to modify the characteristics of water, thereby transforming the field of biomedical engineering.

Raman system with DCS 120 scan head

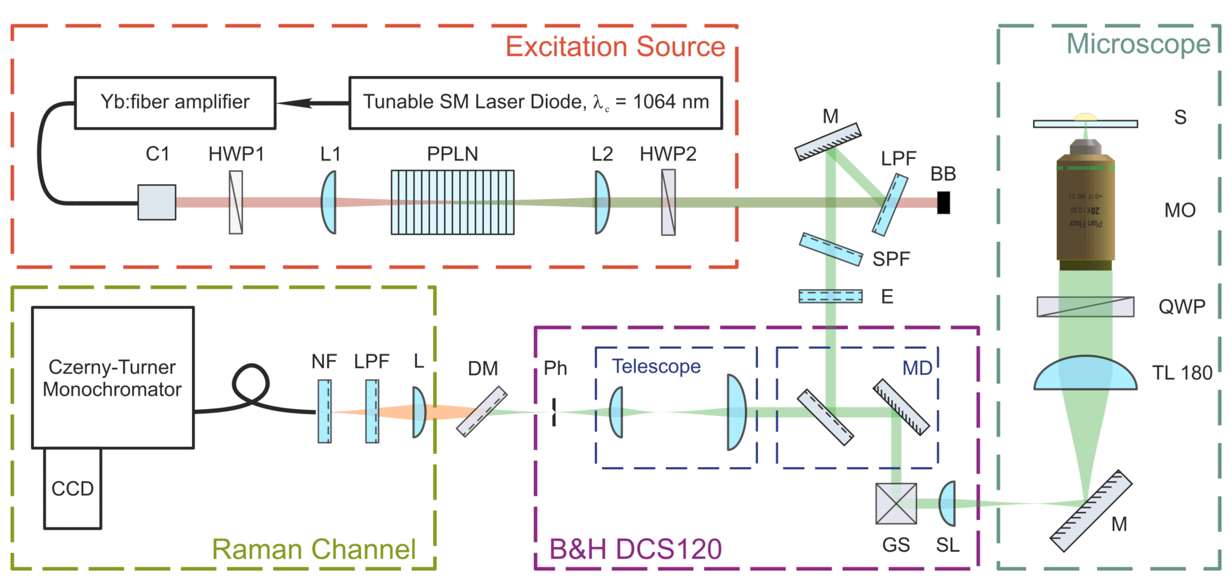


Figure 1. Raman Spectroscopy setup

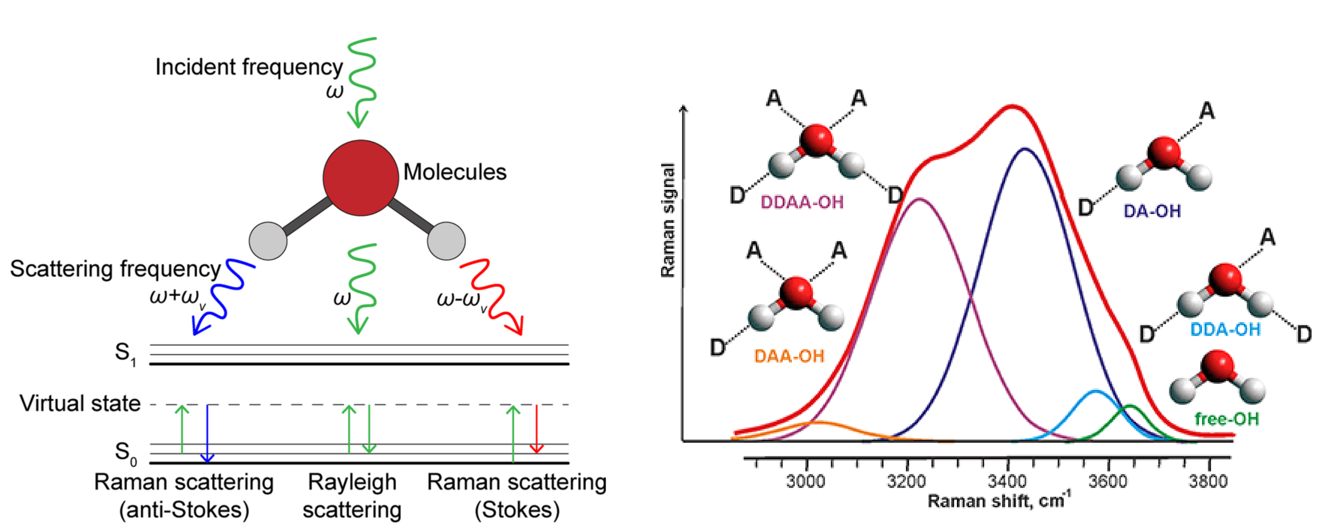


Figure 2. a) Raman Spectroscopy Principle
b) Raman Spectrum of Water

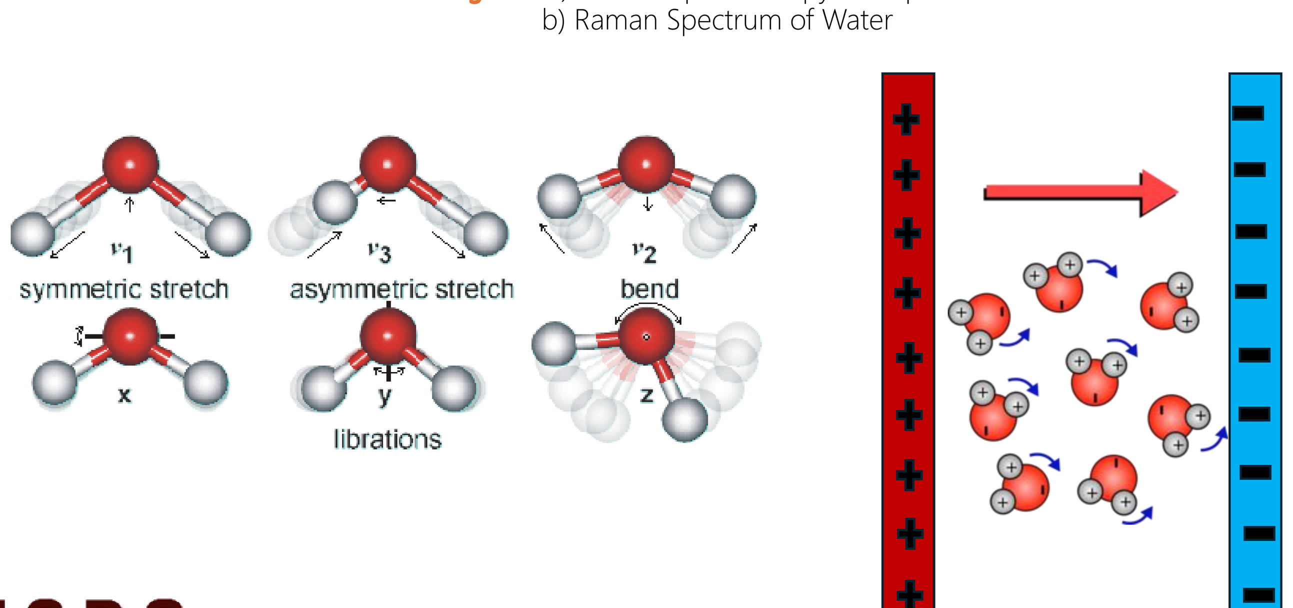
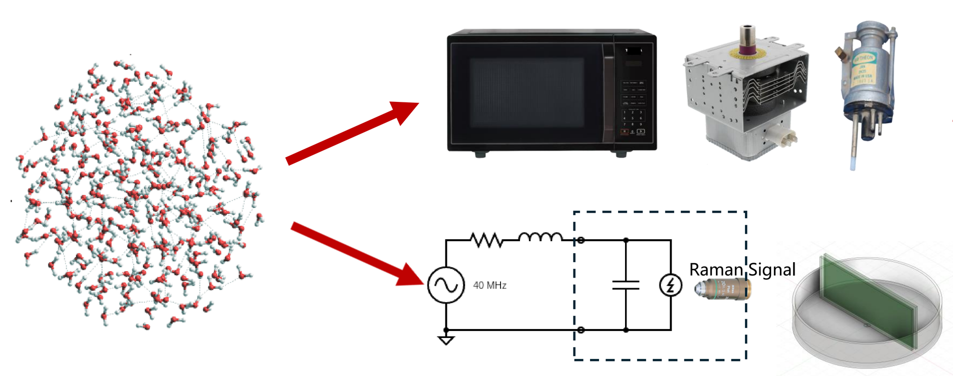


Figure 3. a)Water Vibration Modes
b)Water Molecules Aligned with Electric Field

Methods

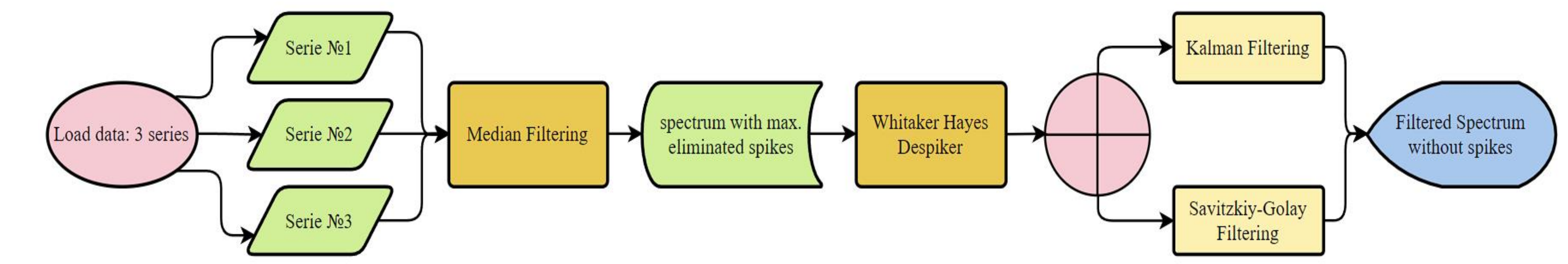
An infrared laser beam with a wavelength of 1064 nm was used as initial excitation source, and it was later converted inro 532 nm green beam using a second harmonic generation process in BBO crystals. To acquire the Raman spectra of the water molecules, this 40–50 mW 532 nm beam was used as an excitation source for specimen. With a working distance of 2 mm, a 40x objective was used to focus the laser beam onto the water layer. An ANDOR Newton linear CCD camera, spectrometer, and monochromator were used to gather and examine the Raman scattered light. The software ANDOR Solis was used to manage the data acquisition process. Datasets of spectra are later analyzed and denoised using Python.



$$Z_c = \frac{1}{j\omega C} = -\frac{j}{\omega C}$$

$$C = \frac{\varepsilon\varepsilon_0 S}{d}$$

$$|\mathbf{E}_{max}| = \frac{V_{max}}{d}$$



Whitaker Hayes Algorithm

let $I_1, I_2, I_3, ..., I_n$ ($n_{max} = 2044$ for camera) are values of Intensity at each wavenumber.

$\nabla I_t = I_t - I_{t-1}$, so that $(t = 2, ..., n)$ form detrended differenced series from this $\mathrm{M} = \mathrm{median}\{\nabla I_t\}$ and $\mathrm{MAD} = \{|\nabla I_t - M|\}$ (median absolute deviation)

Modified Z-score :

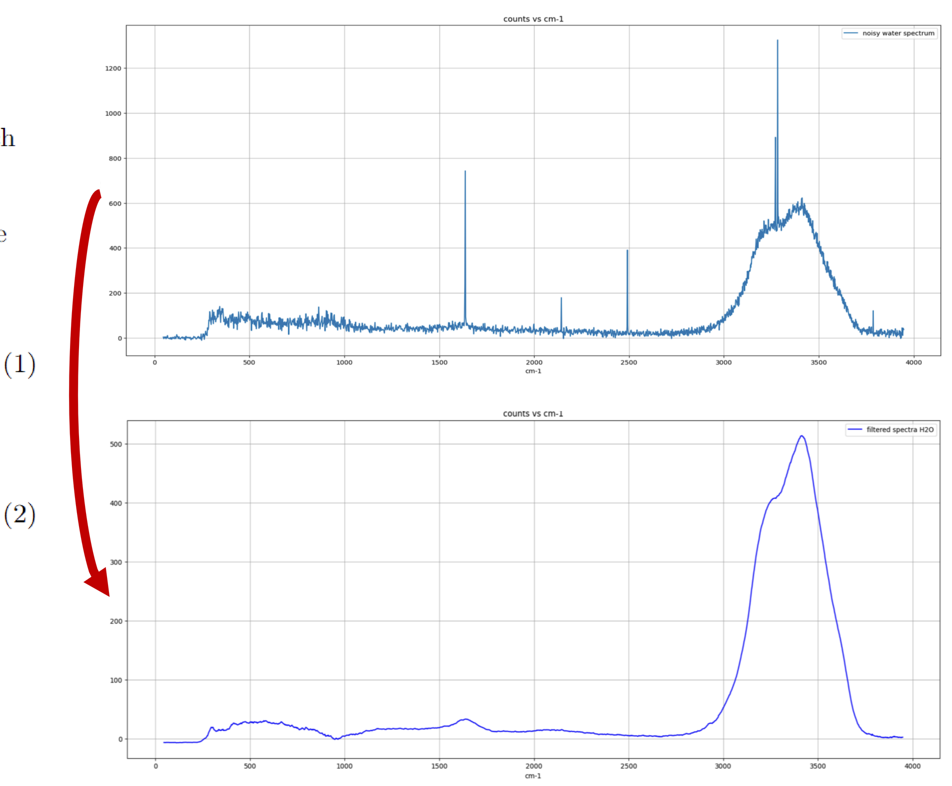
$$Z_t = \mathbf{median}\{\frac{0.6745 \times (\nabla I_t - M)}{MAD}\} \tag{1}$$

where $|Z_t| > 3.5$ is basis of an outlier-labeling rule

$$\tilde{Y}_t = \frac{1}{w}\sum_{t+m}^{t-m} I_t \times \mathbb{I}(|Z_t| < \tau) \tag{2}$$

$$\text{where } \mathbb{I}(u) = \begin{cases} 0, u = False \\ 1, u = True \end{cases}$$

$$\text{and, } w = \sum_{t+m}^{t-m} \mathbb{I}(|Z_t| < \tau)$$



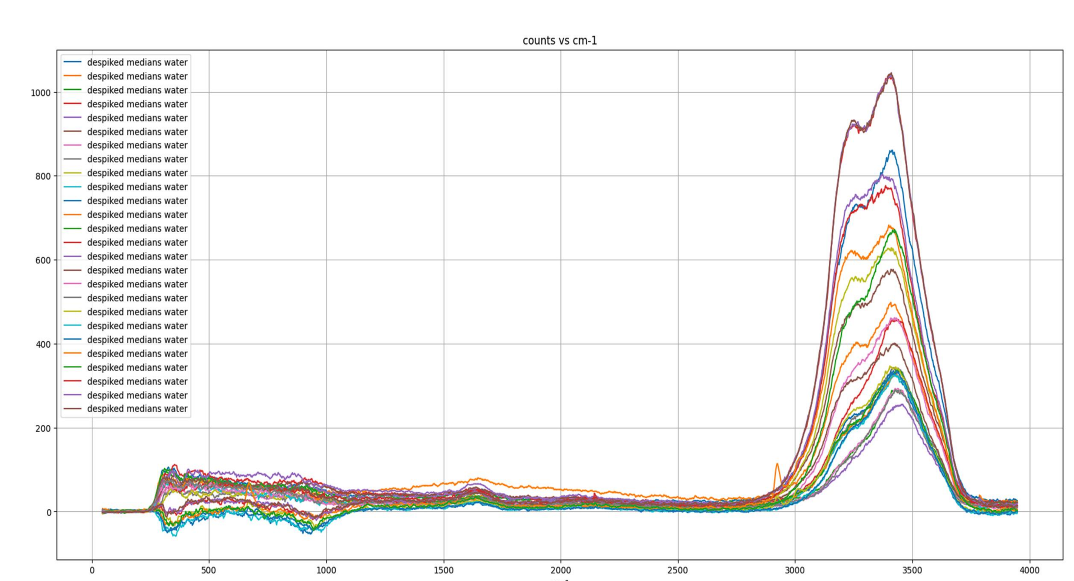


Figure 4. Pure water spectra at normal conditions

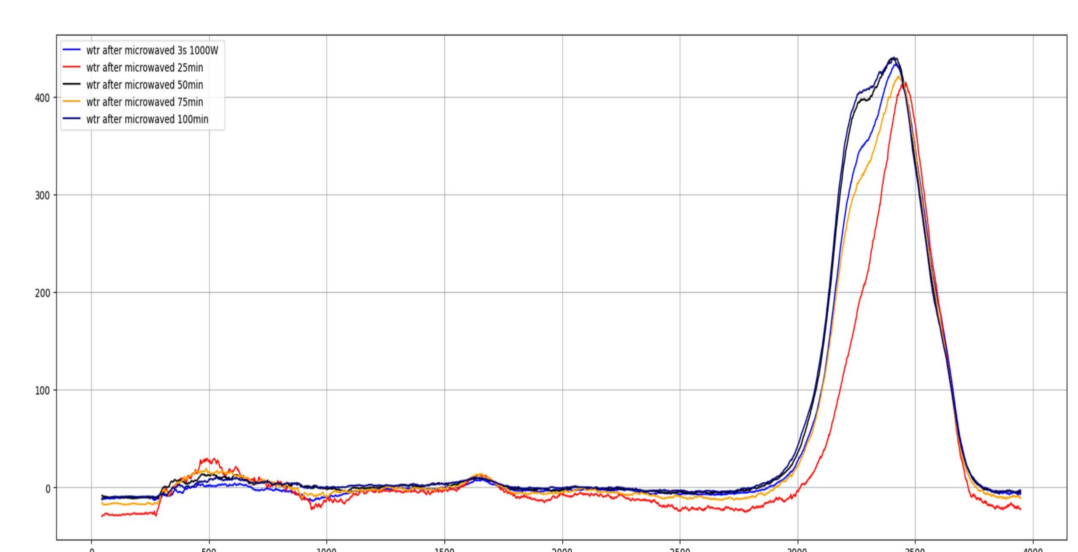


Figure 5. Spectra Transformations after 3s exposure to Microwaves

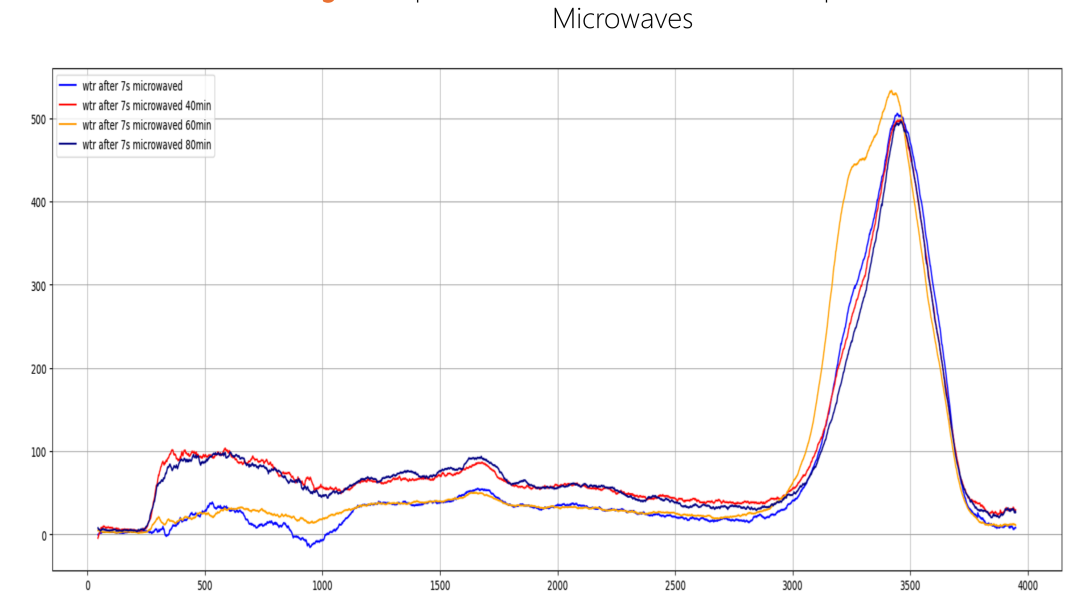


Figure 6. Spectra Transformations after 7s exposure to Microwaves

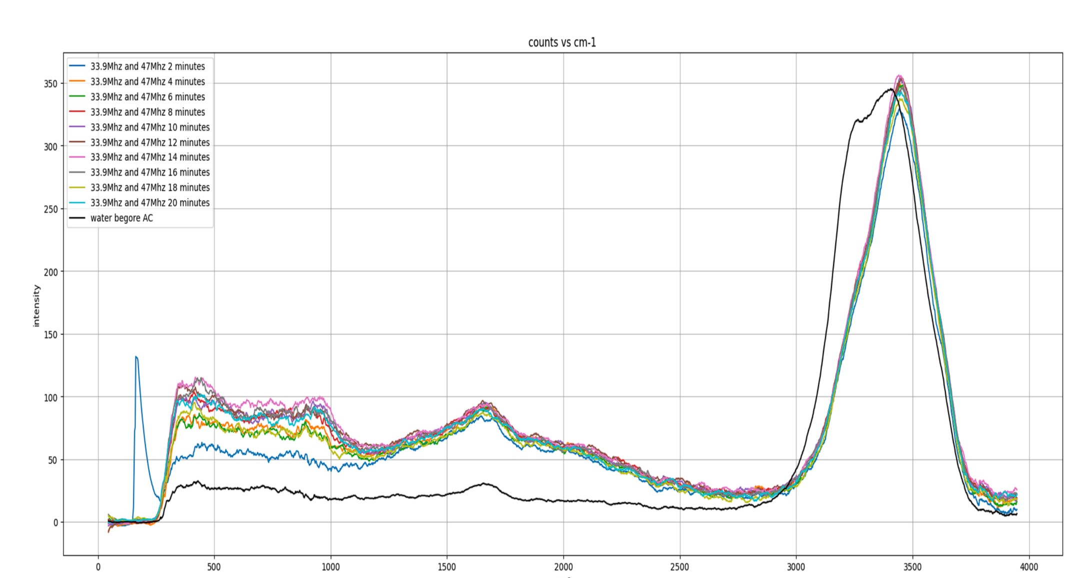


Figure 7. Spectra Transformations in 20 minutes under combined 33.9MHz and 47MHz waveform

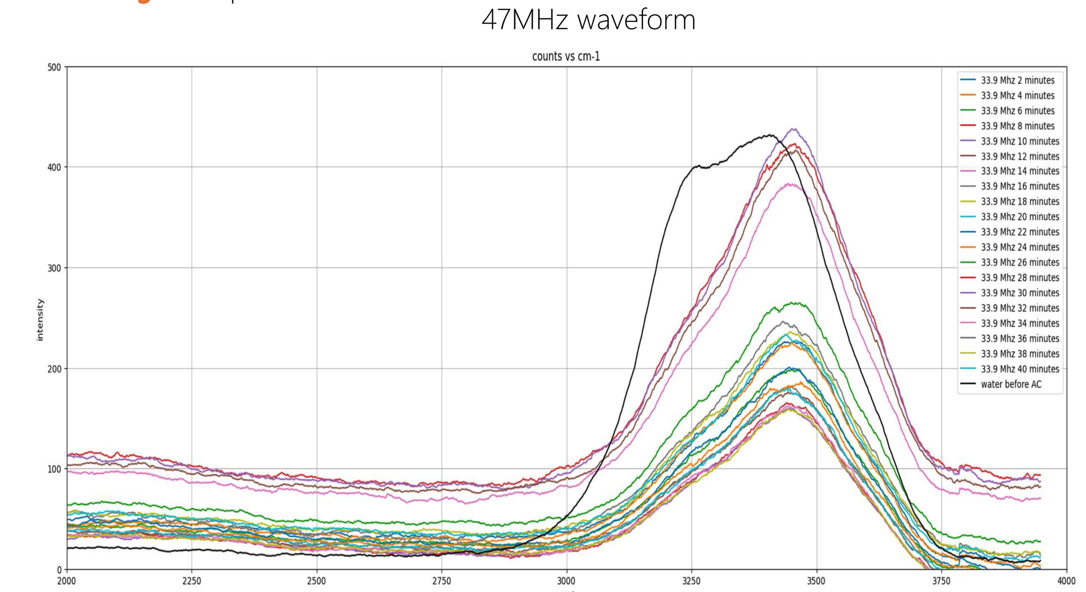


Figure 8. Spectra Transformations in 40minutes under 33.9MHz Alternating Field

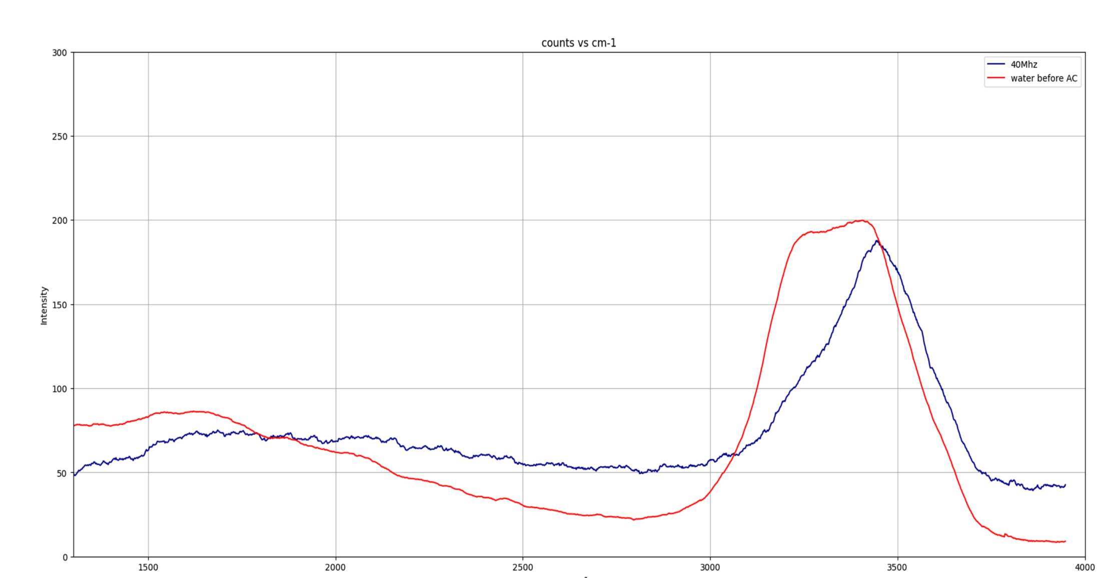


Figure 9. Spectrum Transformation under 40MHz Alternating Field

Conclusion

This study demonstrates that water clusters can be successfully produced in microwave ovens for brief periods of time, as well as in a specially constructed system using an alternating electric field. These discoveries hold great promise for controlling hydrogen bonds in proteins, DNA, and other essential biomolecules, with potential uses in molecular biology and biomedical engineering. To ensure the accuracy of our results, we also evaluated the effectiveness of popular filtering and smoothing algorithms for processing raw noisy data. This work opens up new avenues for the manipulation of molecular interactions and water properties, resulting in substantial advances in both scientific research and technological applications.

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References

K. E. Otto, M. Z. Xue, P. Zielke and M. A. Suhm, "The Raman spectrum of isolated water clusters," *Physical Chemistry Chemical Physics,* vol. 16, no. 21, pp. 9849-9858, Jun. 2014. https://doi.org/10.1039/c3cp54272f

S. Laurette, A. Treizebre and B. Bocquet, "Hydration layers of alcohol and proteins analyzed by THz BioMEMS," *Proceedings of the 14th International Conference Miniaturized Systems for Chemistry and Life Sciences,* Groningen, The Netherlands, pp. 1964-1966, Oct. 2010. [Online]. Available: https://www.rsc.org/binaries/loc/2010/pdfs/Papers/668_0152.pdf

F. Perakis et. al., "Vibrational Spectroscopy of Water," *Chemical reviews*, vol. 116, no. 13, pp. 7590-7607 Apr. 2016. https://doi.org/10.1021/acs.chemrev.5b00640

H. J. H. Geesink, I. Jerman and D. K .F. Meijer, "Water, The Cradle of Life via its Coherent Quantum Frequencies," *Water,* vol. 11, pp. 78-108, Apr. 2020. http://dx.doi.org/10.14294/WATER.2020.1

C. Choe, J. Lademann and M. E. Darvin, "Depth profiles of hydrogen bound water molecule types and their relation to lipid and protein interaction in the human stratum corneum *in vivo," Analyst,* vol. 141, pp. 6329–6337, Oct. 2016. http://dx.doi.org/10.14294/WATER.2020.1

D. Whitaker and K. Hayes, "A simple algorithm for despiking Raman spectra," *Chemometrics and Intelligent Laboratory Systems,* vol. 179, pp. 82-84, Aug. 2018. https://doi.org/10.1016/j.chemolab.2018.06.009

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