The Auditory Evaluation of Chemical Spectra and its Application in Exploring an Alternative User Interface

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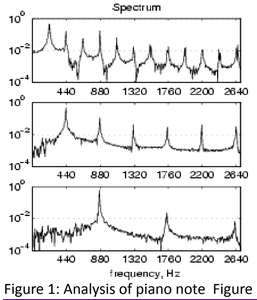
INTRODUCTION

There are a variety of scientific spectroscopies such as Infrared Spectroscopy, Nuclear Magnetic Resonance Spectroscopy , and X-Ray Fluorescence used to study matter and processes. These each use distinct segments of the electromagnetic spectrum, and each has signals observed over a range of frequencies in its segment. A plot of the intensity of these signals vs. frequency often looks similar to an audio signal frequency plot. It should therefore be possible to mathematically convert a chemical spectral analysis into a sound, one which can be recreated through music software. Figure 1 and 2 below are examples of two different frequency spectra. Both spectra have distinct peaks as well as residual noise, the difference being that the Frequency in Figure 1 is measured in Hz and that in Figure 2 is measured in ppm. If we convert the raw data in Figure 2 from ppm to Hz we should find even more similarities between the two frequency plots and possible distinct auditory trends between functional groups. One of my main goals after determining if there are distinct auditory trends between frequencies and different types of compounds and if they can be related back to musical notes on a piano or other musical instruments, would be to look at the practical application of sound within a laboratory setting. By bringing sound into a field dominated primarily by sight and smell, we could revolutionize the field and bring in new minds.



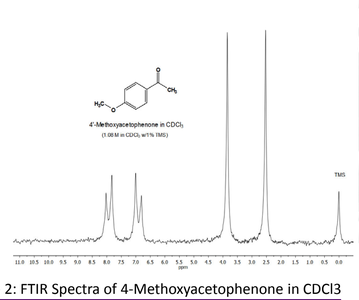


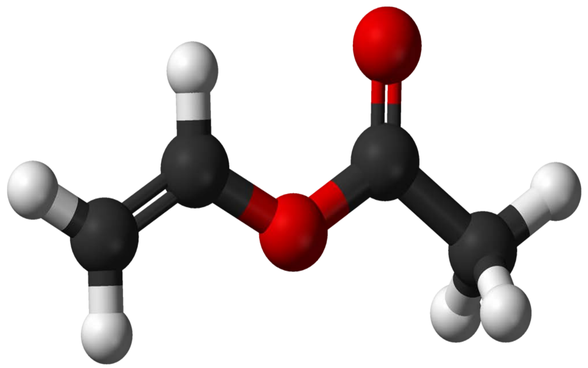
Figure 1: Analysis of piano note Figure 2: FTIR Spectra of 4-Methoxyacetophenone in CDCl3

METHOD & MATERIALS

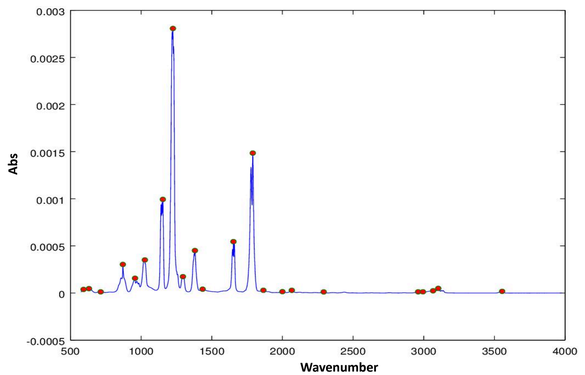
Two Approaches to converting spectral signals to sound: first; use published FTIR conversion software and extend it to additional spectral methods. This would require code analysis and modifications. OR Acquire our spectra in digitized format, as an x vs. y table, and create a conversion algorithm to change the spectral frequency range into the audible range. The absorbance values are equivalent to sound loudness. The x-axis is converted by a linear scaling algorithm. For some spectra like XRF it may be needed to use a non-linear function to “spread out” the low frequencies (low energy absorbance). Software expertise was sought to change the excel data output to sound on the computer. We have been using The NIST Quantitative Infrared Database as well as data off of our own Infrared Spectrophotometer to run through the software as well as analyze the process.

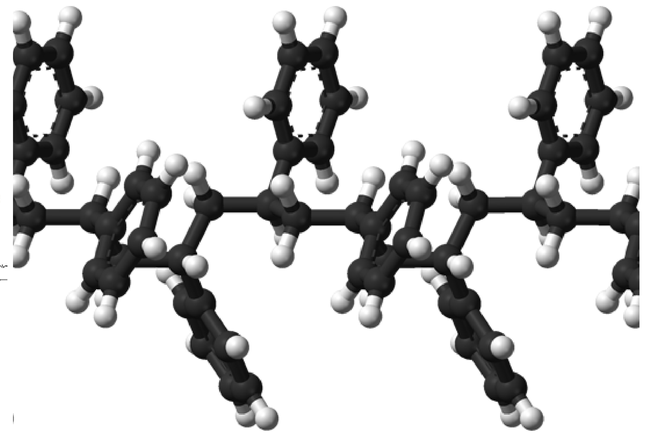
Discussion

Vinyl Acetate



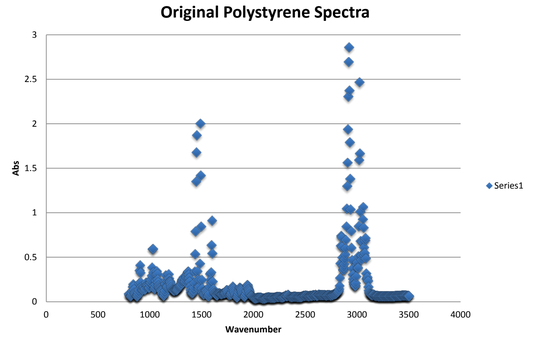
The IR Spectra of Vinyl Acetate within Octave using Peak Picking

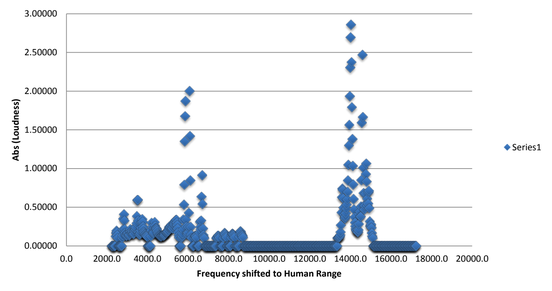




Polystyrene

Original Polystyrene Spectra





Excel Graph representation of Polystyrene in Hz.

Table of Frequencies as Used in Music

Numbers 0-8 represent the octave level. Each note value is shown along with its respective frequency value. The unit of measure is hertz (Hz). The frequency values are based upon A=440 Hz and where middle C is valued at the C4 level or 262 Hz.

0	1	2	3	4	5	6	7	8
Value	Value	Value	Value	Value	Value	Value	Value	Value
C 16	C 33	C 65	C 131	C 262	C 523	C 1047	C 2093	C 4186
C# 17	C# 35	C# 69	C# 139	C# 278	C# 554	C# 1109	C# 2218	C# 4435
D 18	D 37	D 73	D 147	D 294	D 587	D 1175	D 2349	D 4699
D# 20	D# 39	D# 78	D# 156	D# 311	D# 622	D# 1245	D# 2489	D# 4978
E 21	E 41	E 82	E 165	E 330	E 659	E 1319	E 2637	E 5274
F 22	F 44	F 87	F 175	F 349	F 699	F 1397	F 2794	F 5588
F# 23	F# 46	F# 93	F# 185	F# 370	F# 740	F# 1475	F# 2960	F# 5920
G 25	G 49	G 98	G 196	G 392	G 784	G 1568	G 3136	G 6272
G# 26	G# 52	G# 104	G# 208	G# 415	G# 831	G# 1661	G# 3322	G# 6645
A 28	A 55	A 110	A 220	A 440	A 880	A 1760	A 3520	A 7040
A# 29	A# 58	A# 117	A# 233	A# 466	A# 932	A# 1865	A# 3729	A# 7459
B 31	B 62	B 124	B 247	B 494	B 988	B 1976	B 3951	B 7902

Results

We were successful in taking data acquired with our FTIR and importing the data into Octave with an auditory outcome.
Software limitations on the NMR and XRF are hindering the direct transfer of data into Octave at this time.

CONCLUSIONS

We have not found any auditory trends yet, but we think that we are going to end up looking for specific chords instead of each singular note corresponding to a specific functional group .
- Functional groups have ranges for where they could appear on IR spectra and those ranges can over lap.

We are also looking into a more automatic way to convert the raw data from the spectra into excel or into Octave.
- Not using Octave will give us more control on which peaks are being used.

REFERENCES

Valsler, Ben. "The Music of Molecules." Web log post. *Chemistry World Blog*. N.p., 4 June 2014. Web. 17 Mar. 2015. <http://prospect.rsc.org/blogs/cw/2014/06/04/the-music-of-molecules/>.

Pereira, Florbela, João C. Ponte-e-Sousa, Rui P. S. Fartaria, Vasco D. B. Bonifácio, Paulina Mata, Joao Aires-de-Sousa, and Ana M. Lobo. 2013. “Sonified Infrared Spectra and Their Interpretation by Blind and Visually Impaired Students.” *Journal of Chemical Education* 90 (8): 1028–31. doi:10.1021/ed4000124.

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