A Molecular Musical Instrument

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1 Introduction

We designed a web app which allows the user to "play" molecules as musical instruments. Using infrared spectroscopy data, we calculate the fundamental vibrational frequency of each atom within the molecule, which corresponds to pitch. We extract other molecular parameters, which map to the other characteristics of the molecule's distinct sound. This allows us to build a visual and auditory intuition for chemical properties.

2 Theory

We start by approximating the attractive force between two molecules as proportional to the displacement between the molecules, aka the bond radius r.

$$F = -kr$$

This also gives us the potential energy of the bond:

$$U(r) = -\int F\,dr \; = \frac{1}{2}kr^2$$

Molecules have vibrational modes, or patterns of vibration, each of which is associated with a quantum number v. When molecules are excited (typically in the mid-IR range), they jump from quantized energy levels. Each of these energy transitions is associated with a unique frequency and unique vibrational pattern.

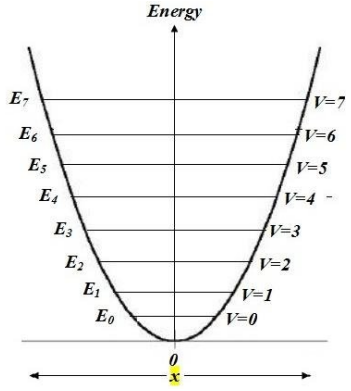

Figure 1: Simple Harmonic Approximator for U(r)

In fact, this simple harmonic approximation aligns well with the experimentally determined graph for bond potential energy. This is especially true when we remain local to r_e, the value of r for which $U(r)$ is minimized. Here's a graph that might look familiar:

As bond length deviates from r_e, we observe anharmonic behavior (more complex then the harmonic approximation). As $r \to 0$, and the molecules draw closer and closer together, $U(r)$ goes to infinity. As

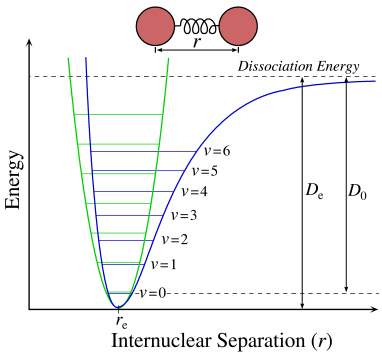

Figure 2: Anharmonic Oscillator for U(r)

$r \to \infty$, and the molecules drift apart, $U(r)$ tapers off around an asymptote. This is what we expect from the theory of internuclear separation.

The energy transition $v = 0 \to v = 1$ produces the fundamental frequency, which is purely harmonic. Other transitions associated with $\Delta v = \pm 1, 2, 3, ...$ produce overtone frequencies, which are anharmonic. The first overtone is slightly less than $2 \cdot fundamental$, the second overtone is even further less than $3 \cdot fundamental$, etc.

3 Building the App

3.1 Frequency Data

To generate frequency data, we ran simulations based on molecular geometry using Psi4, a Python package dedicated to quantum chemistry calculations. The package runs multiple iterations, for each of the possible geometric configurations for a molecule. In each iteration, it calculates the molecule's vibrational energy and wavefunction. From the wavefunction, we can extract the fundamental frequency for each vibrational mode.

3.2 Additional Chemical Properties

We selected two other properties to map to other sound parameters. We mapped molecular weight to timbre, such that heavier molecules have a "darker" sound. We also mapped hydrogen donor strength to a low-pass filter, such that molecules more eager to donate hydrogen atoms have less filter–they get to the point quicker.

3.3 Creating Sounds

We used MIDI to create sounds of specific frequency and timbre per these specifications, with one distinct sound per vibrational mode. We converted to .wav files to apply the low-pass filter, and finally to .mp3 to easily play in the web browser.

3.4 Visualization

In order to visualize vibrations, we found files online generated from IR spectroscopy of the following molecules: H_2O, CO_2, H_2, and C_2H_4. Using PyMol and PyVibMS (two Python visualization packages), we created .gif files showing the distinct vibration for each of the molecule's modes.

3.5 Building the App

We built the web app using HTML, JS, and CSS. It accepts the molecule and vibrational mode as input, and in turn displays the vibrating molecule with its corresponding sound. In the future, we hope to add the ability to play multiple molecules at once, as well as to play any molecule beyond the four we have collected data on.

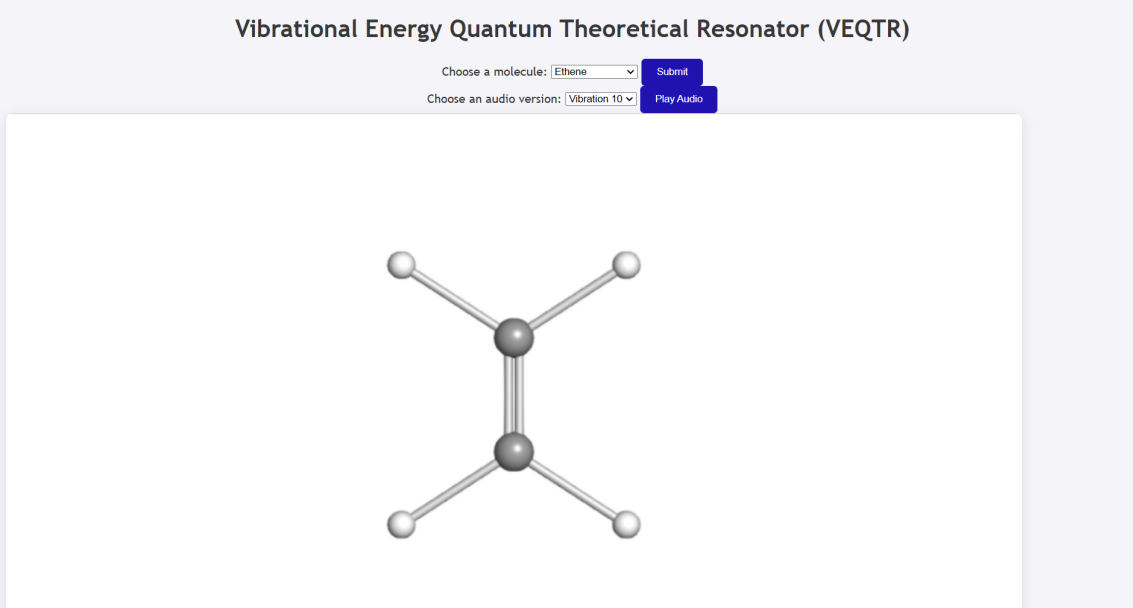

Figure 3: Web app displaying vibrational mode 10 of ethene

4 Reflection

I really enjoyed this project as an opportunity to explore a side of molecular motion I had never considered before–vibrations. Connecting it to music proved a fun way to build an intuition for motion. I also developed web development skills, which is always a plus! :)

5 Works Cited

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