Spectroscopy

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Abstract

The structure and composition of a molecule can provide useful information for chemists to learn about mechanisms and reactions. However, it is impossible to physically see the atoms and bonds in a compound. In order to determine what the molecule is and get an idea of its structure, scientists use various forms of spectroscopy.

This project will demonstrate some of the molecule vibrations that cause the various results seen in a spectroscopy spectrum. VPython will be used to create the atoms and bonds and simulate their bends and stretches, which are mainly seen in infrared spectroscopy (IR).

1 Background

In chemistry, spectroscopy is often used to identify a molecule in order to determine unknown compounds and impurities in samples. There are different types of spectroscopy that one can use. Each has its own advantages and disadvantages, which depend on the main end goal of the chemist.

1.1 Infrared Spectroscopy

One type is *infrared spectroscopy* (IR), often used to analyze samples with covalent bonds. This uses infrared radiation, with long wavelengths and lower frequencies, to analyze a compounds functional groups. Peaks and bands in an IR spectrum represent absorbed wavenumbers, or the resonant frequency at which the absorbed energy matches the transition energy of the bond or functional group vibrating. When the bonds are disturbed, they vibrate in quantized modes, bending and stretching, giving off quantized energy in packets.

There are different ranges of infrared on the electromagnetic spectrum: *near*-, *mid*-, and *far*-infrared, all relative to the visible spectrum. High energy *near*-IR can excite overtone or harmonic vibrations. *Mid*-infrared, one of the most commonly utilized regions, can be used to analyze fundametnal vibrations and their rotational vibrational structure. The *far*-infrared is very low energy, and can be used for rotational spectroscopy.

Unfortunately, IR can only provide qualitative information, not necessarily quantitative information such as how many bonds are present. However, it is a quick, reliable, and cost efficient technique to analyze a sample, which is why it is widely used in research and industry in both organic and inorganic chemistry. They are a great way to test for impurities in a product, as they are fairly sensitive.

1.2 Nuclear Magnetic Resonance Spectroscopy

A type of quantitative spectroscopy commonly used is *nuclear magnetic resonance* (NMR). It utilizes the magnetic properties of certain atomic nuclei, applicable to any containing spin properties. There are different types of NMR that can be utilized. One common method to help with determining a small organic molecules structure is proton NMR (^{1}H-NMR). Evaluating an NMR spectrum means one has to take into account unique proton environments (symmetry), chemical shift, multiplicity, and integration.

If there is symmetry within the molecule, those protons will typically be considered one group. Depending on whether there are electron withdrawing atoms nearby the protons or whether they are in an alkane chain, shielding can come into effect for the chemical shift; downfield means they are more deshielded, with electron withdrawing groups pulling the electron cloud away from the protons, and upfield means they are more shielded, such as those in an alkane chain. This can lead to conclusions about the relative placement of some of the proton groups. Multiplicity and integration allow one to see how many protons are within a group and how many are nearby that group, giving some more idea of a general structure of the molecule.

There are different types of NMR that can be used, depending on the compounds being evaluated. Carbon NMR (^{13}C-NMR) can also be used, but is only necessary if there are few identifiable C-H bonds within a molecule. It is much less sensitive than proton NMR, and thus needs a more concentrated sample. For some larger, more complex compounds, phosphorous NMR (^{31}P-NMR) is also less sensitive than ^{1}H-NMR, but better than carbon NMR. It has a large chemical shift range, and shows sharp peaks. However, it does not contribute much to the structure of the molecule. Rather it is used to determine a large, complex compound's identity.

NMR is very useful to identify organic compounds. However, it is not the best test for determining impurities in a sample, as it is not the most sensitive method of analyzing a compound. The spectrometers themselves are very expensive, and thus they are not commonly found outside of universities.

2 Goals

Although I have very little background in programming, I hope to stimulate the types of bond stretches and bends analyzed by IR spectrum in VPython. There are different types of stretches (symmetric and asymmetric) and bends (twisting, wagging, rocking, and scissoring) that can be represented by a moving ball-and-stick model, which is similar to a stationary molecular model kit. With this formatting, I can likely use a blobbyman style to create the atoms and bonds that need to move. If I can master the basic CH_2 model stretches and bends, then I may move on to create more complex bonds.

3 Timeline

October 31: Get VPython working on my computer
November 11: Create the stationary CH_2 model as the basis of the RTICA
November 18: Move the model's hydrogen atoms the the stretching simulations
December 2: Move the model's hydrogen atoms in the bending simulations
December 9: If I have time, I would like to try modelingl more complex bonds or phenol rings.