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Math198
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Pre-Proposal

Objective:

Create a visual for bond movements within functional groups that can be identified by IR.

Spectroscopy:

Spectroscopy is used by chemists to help identify an unknown compound. There are different types of spectroscopy that can be used to draw various conclusion about a molecule.

One type of spectroscopy is infrared spectroscopy (IR). This uses infrared radiation to analyze a compounds functional groups. Peaks and bands in an IR spectrum represent absorbed wavenumbers, due to the flexibility of the bonds between atoms. When the bonds are disturbed, they vibrate in quantized modes (bending and stretching), giving off quantized energy in packets. Different compounds absorb different wave numbers of infrared radiation to cause certain types of vibrational modes. The lowest region of an IR spectrum, typically between 1500 cm-1500cm-1, is considered the fingerprint region of the spectrum, holding key patterns unique to certain molecules or functional groups. Unfortunately, IR only provide qualitative information, not necessarily quantitative information such as how many bonds are present.

A type of quantitative spectroscopy commonly used is nuclear magnetic resonance (NMR). There are different types of NMR that can be utilized. One common method for helping with determining a molecules structure is proton NMR, or 1H-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. Multiplicity and integration allow one to see how many protons are within a group and how many are nearby that group.

However, proton NMR cannot tell one about the specific functional groups within a molecule, only the placement of protons in a proton rich environment. This is why no one test can be used to identify a compound with certainty, and why several tests must be run. For some larger, more complex compounds, phosphorous NMR (31P-NMR) can be used. However, they can only identify a certain compound based off of previous chemical shift values of known compounds, providing only one distinct peak per compound rather than giving any information about its structure. Carbon NMR (13C-NMR) can also be used,

but does not provide as detailed information as proton NMR either. Only some peaks are well known as being present to indicate certain common functional groups.

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.