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Simulation Tool to Determine Presence of Impurities in an Organic Compound Using IR Spectroscopy

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ABSTRACT

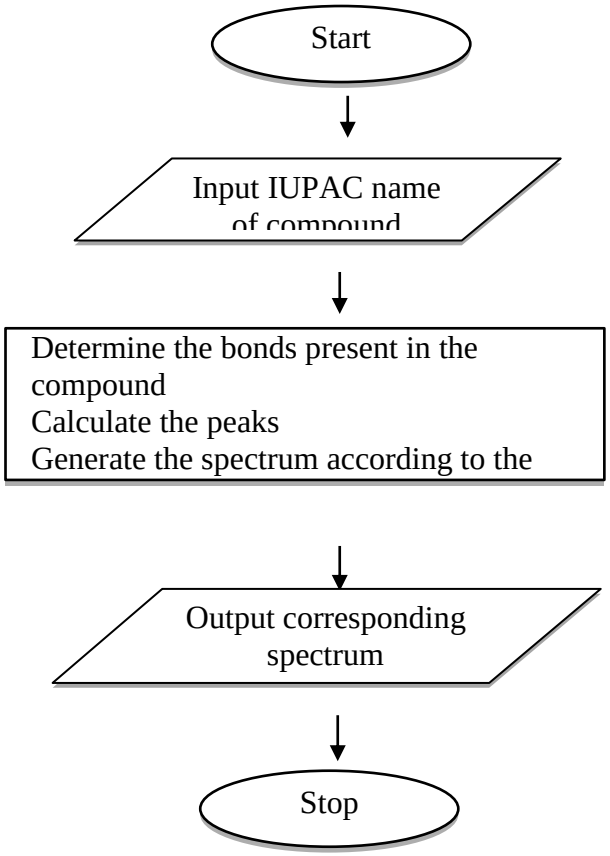
The popularity of using IR Spectroscopy in elucidation of organic and inorganic compounds in both research and industry has driven development of an array of IR Spectral analysis of tools and databases. IR Spectroscopy is used to identify and study the component chemicals. It relies on infrared radiations and can provide detailed information about the structure, dynamics, and functional groups involved. The paper outlines the development of simulation tool to obtain the IR Spectra of the compound by entering its name. The position of the peaks is obtained through interaction of infrared radiation with the various functional groups present in the given compound.

Keywords: IR Spectroscopy, Interaction of IR Radiation with compound.

I. INTRODUCTION

Infrared spectroscopy or commonly known as IR Spectroscopy is based on the Principle that the molecules absorb frequencies that are characteristic of their structure. The absorptions occur at resonant frequencies, i.e. the frequency of the radiation absorbed is similar to the vibrational frequency. The masses of the atoms, the associated vibronic coupling and the molecular potential energy surfaces affect the energies. Various types of bonds respond to the IR radiation differently. For example, triple bonds and double bonds are shorter and stronger than single bonds, and therefore vibrate at higher frequencies. The types of atoms involved in the bonds are also relevant. For example, O-H bonds are stronger than C-H bonds, so O-H bonds vibrate at higher frequencies. Therefore various functional groups present in the compound can be identified using IR spectroscopy. IR radiation is absorbed only in presence of the dipole moment. In general, the stretching frequency of a bond which has a dipole moment, causes the absorption in IR spectrum. If the bond is symmetrically substituted, has zero dipole moment, its stretching vibration is very weak or absent in the spectrum (IR-active v/s IR-inactive vibrations). Molecular collisions, vibrations and rotations cause change in symmetry in bonds with zero dipole moment and thus produce weak absorptions. The objective of our tool is to generate a theoretical IR Spectrum which can be used to compare with the experimental graph that is obtained when Infrared radiation is allowed to pass through an organic compound prepared in the laboratory.

II. METHOD

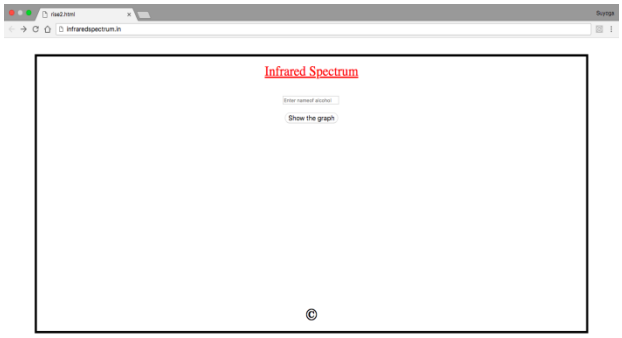


The flow chart shows the procedure to determine the theoretical IR spectrum merely based on the information about the functional groups available. First, the IUPAC name of the compound has to be given as input to the simulation tool. After the data corresponding to respective peaks are fetched from the database, the graph between transmittance v/s wave number. The spectral lines of theoretical data and sample are compared. After comparison, a conclusion can be drawn regarding the presence of impurities. If the spectral lines are same then we can say that there are no impurities present otherwise we say there are some sort of impurities present.

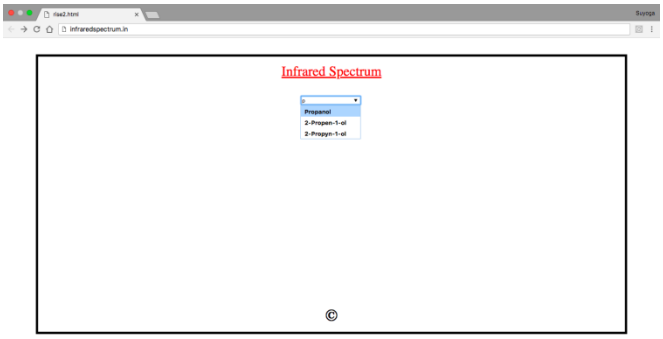
III. RESULTS AND DISCUSSION

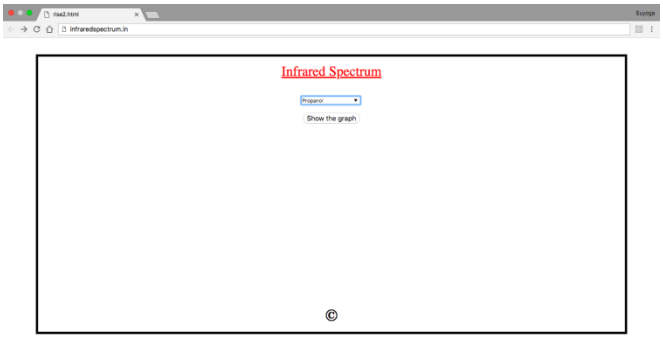
An example can be considered to observe how the peaks can be obtained

Step 1. Open the webpage.



Step 2. Enter the compound.
The compound can be either entered by name or by selecting desired compound from dropdown box.
Here the dropdown box is shown.



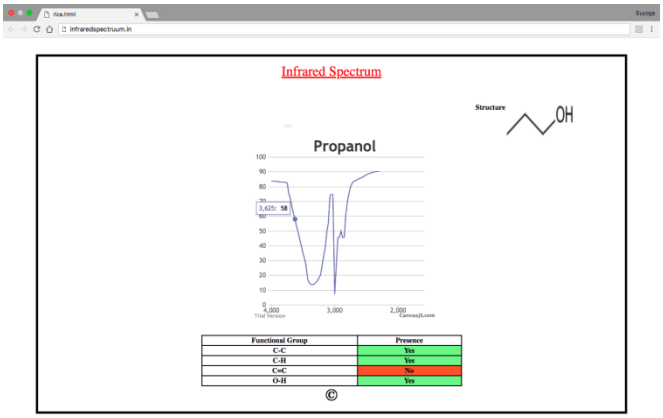


Here, the name of the compound is entered through keyboard.
Propanol is selected/entered.

Step 3. Spectrum is displayed.

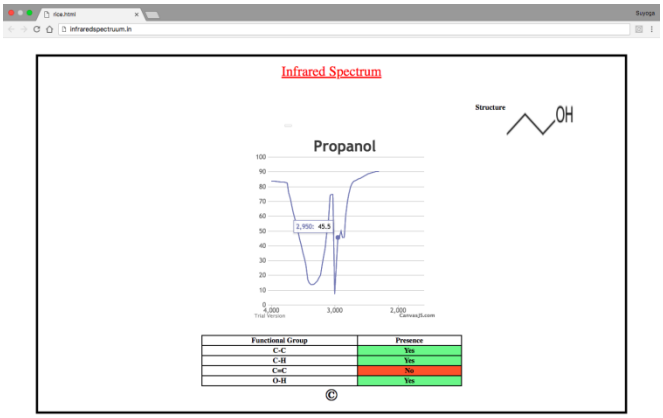
If a valid compound is entered, the bonds present are found out, hence the peaks are calculated. Structure, a table containing the bonds present and the spectra are displayed.

As propanol is entered, table, structure and spectra of propanol is displayed.

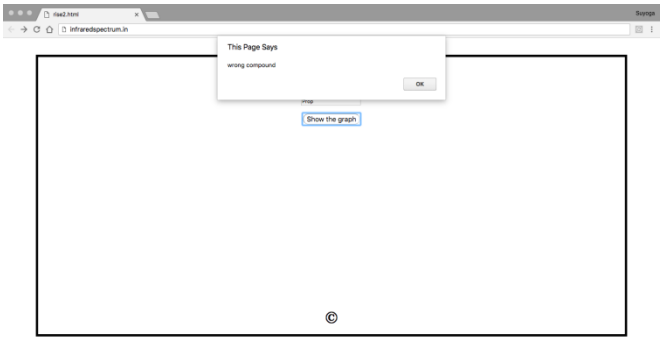


On moving the cursor along the spectra, wavenumber and its corresponding absorbance can be determined.

In the case below, the cursor is moved to the wavenumber 2950. Its corresponding absorbance 45.5 is shown



If a wrong compound is entered, user is alerted by a display stating a wrong compound has been entered.



IV. CONCLUSION

1. For finding impurities in pharmaceuticals: Several regulatory authorities like the International Conference on Harmonization (ICH), the United States Food and Drug administration (FDA), and the Canadian Drug and Health Agency (CDHA) are accentuating on the purity requirements and identifying impurities in Active Pharmaceutical Ingredients (APIs) .
2. For obtaining pure organic compounds in the chemistry laboratory for amateur experiments.

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VI. REFERENCES

[1]. https://webbook.nist.gov/chemistry
[2]. https://en.wikipedia.org/wiki
[3]. Elementary Organic Spectroscopy by YR Sharma