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Electronegativity Effect on C-Halogen Bond Stretching in Alkyl Halides at Higher Education Level

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Abstract

Electronegativity is an intrinsic parameter of each chemical element that influences the response, chemical reactivity, polarity, as well as the attraction between molecules among other effects. In this sense, a didactic strategy was developed for teaching at the undergraduate level to determine the effect that electronegativity has on the vibration response of the C-Halogen bond in a molecule, through a practical experience that involved on the one hand the technique of infrared spectrophotometry and organic molecules with the presence of halogen atoms. The didactic strategy was applied to a group of students of the bachelor's degree in industrial chemistry, which was divided into teams of 5 students who worked based on cooperative learning and with problem-based learning support, they were studying spectroscopy and who had previous knowledge of the infrared spectroscopy technique. After carrying out, the experiment and with the results obtained, the students were able to conclude that due to the strength and distance of the bond between halogen and carbon, the value of the wavenumber (cm^{-1}) is modified, concluding that in shorter bonds a greater energy is required for it to be stretched and in longer and weaker bonds as in the case of Iodine these are stretched to a lower wavenumber. This allowed students to understand this phenomenon and the dependence of electronegativity, bond length, and bond strength on a specific response observed using infrared spectroscopy.

Keywords: Electronegativity, Infrared spectroscopy, Halo alkane, Didactic strategy

1. Introduction

Alkyl halides are also known as halo alkanes or alkyl halides (Wade & Simek, 2016), this type of hydrocarbons present the substitution of one or more hydrogen atoms by an atom of the halogen family such as: Fluorine, Chlorine, Bromine or Iodine, which have electronegativity values than the rest of the chemical elements. Therefore, they have a greater tendency to attract electrons to their nucleus, this tendency increases from left to right and bottom to up, so the electronegativity in this family is F > Cl > Br > I (Figure 1).

As we move up the periodic table from Fluorine to Iodine, the molecular size increases. As a result, we also see an increase in link length. Conversely, as the molecular size increases and we get longer bonds, the strength of those bonds' decreases (Benson, 1965). Alkyl halides fall into different classes depending on how the halogen atom is located in to the carbon chain and can be classified as primary, secondary, or tertiary depending on the alkane to which they are attached. The chemical reactivity of alkyl halides is frequently discussed using alkyl halide classifications to help discern patterns and trends (Colthup et al., 1990). Because the binding pattern for halogens is one bond and three solitary pairs, carbon and halogen always share a single bond. The classification of alkyl halides is determined by the binding pattern of the carbon atom attached to the halogen as shown in the diagram below.

The aim of this work is to evaluate at the teaching level the effect exerted by the electronegativity of a halogen on the wavenumber associated with the stretching of the C-Halogen bond. Determining if there is a correlation between the wavenumber of this vibration shown in an IR spectrum and the theoretical electronegativity (Silverstein et al.,

1991). As activities prior to the proposed experimental development, students will investigate the solubility of halo alkanes, as well as the value of the wavenumber reported in the literature for the C-Halogen bond. In addition, the value of the electronegativity associated with the atoms of F, Cl, Br, I to the physical and chemical properties of a family of halo alkanes and the reagents used for a correct storage of the waste.

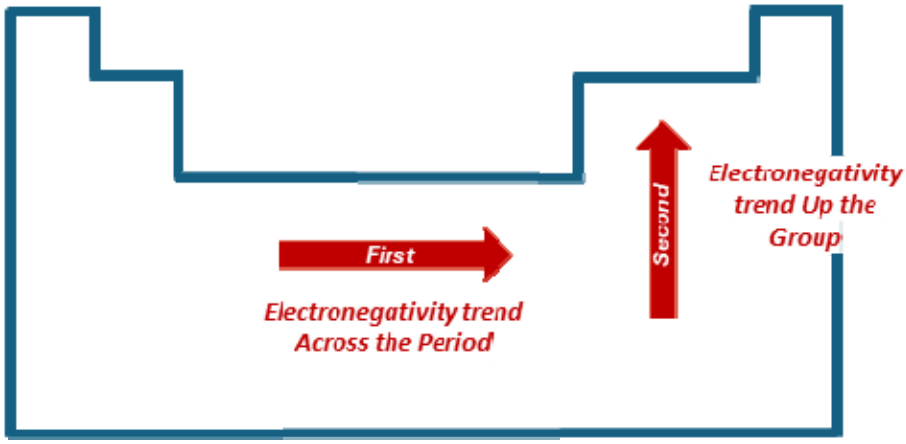


Figure 1. First and second criteria, to assign electronegativity within the periodic table. (Benjamin Velasco-Bejarano's own design)

2. Hypothesis

Electronegativity exerts an important effect on the stretching vibration of the bonds of a molecule shown in an infrared spectrum, so if the wavenumber value for the stretching vibration of the C-Halogen bond in a family of alkyl halides is determined, its effect on them can be observed and assessed.

3. Methodology

To evaluate at the teaching level the effect of the electronegativity of a halogen on the wavenumber associated with the stretching of the C-Halogen bond, a didactic strategy was developed and applied (Castillo et al., 2024) in a group of students of the bachelor's degree in Industrial Chemistry, which was divided into teams of five students who worked based on cooperative learning (Roger & Johnson, 1994) and with problem-based learning support (Groenewald et al., 2023). They were studying the subject of spectroscopy and who had previous knowledge of the infrared spectroscopy technique.

For the experimental determination of electronegativity effect on the stretching of the C-Halogen bond in alkyl halides at the higher education level, a group (2801) of the subject Spectroscopy of the bachelor's degree in Industrial Chemistry of the seventh semester, group 2801 participated composed of 23 students, 43% male and 57% female, with an average age of 21 years.

Previously, the students had reviewed for six weeks the topic of infrared absorption spectroscopy (IR), which was studied through the teacher's explanation using information related to this topic on a Power Point platform, which also included the resolution of typical exercises, as well as discussion of articles (Hemmer & Gasteiger, 2000; Peacock, 2002). Within this unit, the different types of stretches that occur in a bond, both symmetrical and asymmetrical, were reviewed, as well as the influence of intra- and intermolecular phenomena that modify the response in the spectrum of the halo alkane family. The above was done based on the research questions Does electronegativity affect the value of the wave number in a halo alkane? Is the bond distance between C-and different halogens different? In order to answer these questions, the students were asked to experimentally acquire the Infrared spectra of four halogenated compounds (1-Fluoroheptane, 1-Chloroheptane, 1-Bromoheptane, 1-Iodoheptane), as well as the heptane that was used as a reference, as well as the theoretical spectra available in the literature, in order to identify the corresponding differences.

In all cases, an IR spectrum was acquired within a spectral window between 3500 and 400 cm^{-1}, as well as a magnification of IR spectra from 700 or from 1200 to 400 cm^{-1} depending on the halo alkane tested, so that the student could observe the wavenumber values more clearly. It is convenient to mention that, in all IR spectra, the value of the observed band wave number is indicated, which allows the student to identify each of them and associate them with the different types of bonds present in the halo alkane. Additionally, the students were asked to look in the literature for the value of the distance of the C-Halogen bond and its associated energy.

3.1 Material, Reagents and Equipment

The materials, reagents and equipment that were used during the experimental development of this didactic strategy are shown in Table 1, as well as some characteristics of these.

Table 1. Material, regents and equipment used in the methodology previously mentioned

Quantity	Material
• 4 • 4 • 4	• 3 mL vials • Pasteur pipette • Latex bulbs
Quantity	**Reagents**
• 0.5 mL • 0.5 mL • 0.5 mL • 0.5 mL • 0.5 mL	• 1-Fluoroheptane Analytical grade • 1-Chloroheptane Analytical grade • 1-Bromoheptane Analytical grade • 1-Iodoheptane Analytical grade • Heptane Analytical grade
Quantity	**Equipment***
• 1	• Spectrophotometer IR Bruker, Tensor 37 Model

Note. * For the experimental development, a Bruker Tensor 37 equipment was used, this methodology is applicable in any other IR spectrophotometer.

3.2 Procedure

The experimental procedure followed for the acquisition of the spectra of each of the halo alkanes evaluated was described. It is important to mention that students already can acquire IR spectra in an IR spectrophotometer.

(1) Turn on the IR equipment and put it in a position to acquire an ATR spectrum.

(2) They place a 0.5 mL vial of analytical reactive 1-Chloroheptane.

(3) Place 3 drops in the ATR crystal reader in IR equipment.

(4) Acquire the corresponding IR spectra by means of the ATR technique in a spectral window of 3500 to 400 cm^{-1}, and then make an enlargement of the region between 700 and 400 cm^{-1}, or between 1200 and 400 cm^{-1}. Assign the wavenumber values to the observed bands.

(5) Save the file in *pdf format* with the name of the halo alkane analyzed.

(6) Repeat the same operation for 1-Fluoroheptane, 1-Bromoheptane, 1-Iodoheptane and Heptane.

(7) Identify the bands associated with the stretching vibration of C-H, C-Halogen in each of the experimentally acquired spectra.

(8) Make a graph using the value of the experimentally observed C-X vibration and the value of the theoretical electronegativity of each halogen, as well as another between the bond distance and another correlating the bond energy, calculate the correlation coefficient r^2 in each case and discuss the result.

4. Results

The students received the following instructions regarding the integration of the results of this experiment so that they could identify, on the one hand, the value of the C-Halogen stretch wavenumber for each of the four halo alkanes studied, as well as to compare the bands of these with the bands of the heptane used as a reference.

This information will be useful for the student to analyze and make a conclusion about this phenomenon.

(1) Place the acquired infrared spectra (400-3500 cm^{-1} as well as magnification) of the halo alkanes evaluated: 1-Fluoroheptane, 1-Chloroheptane, 1-Bromoheptane and 1-Iodoheptane which must contain in the header date, title, acquisition method, as well as the assignment of the value of the wavenumber of the bands of interest.

(2) Fill in the following table with the theoretical data researched for each of the indicated links.

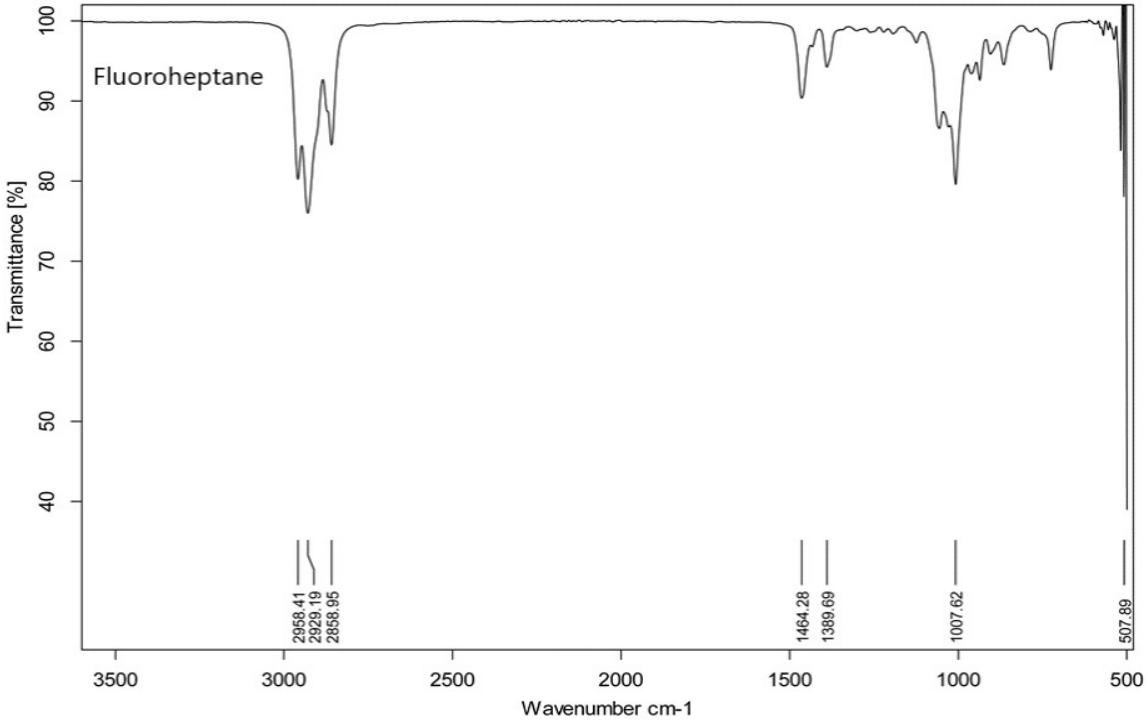
Table 2. Theoretical data for the different carbon-halogen bonds

Bond	**Electronegativity**	**Bond strengths** (kcal/mol)	**Bond length (Å)**
Carbon–Fluorine			
Carbon-Chloride			
Carbon-Bromine			
Carbon-Iodine			

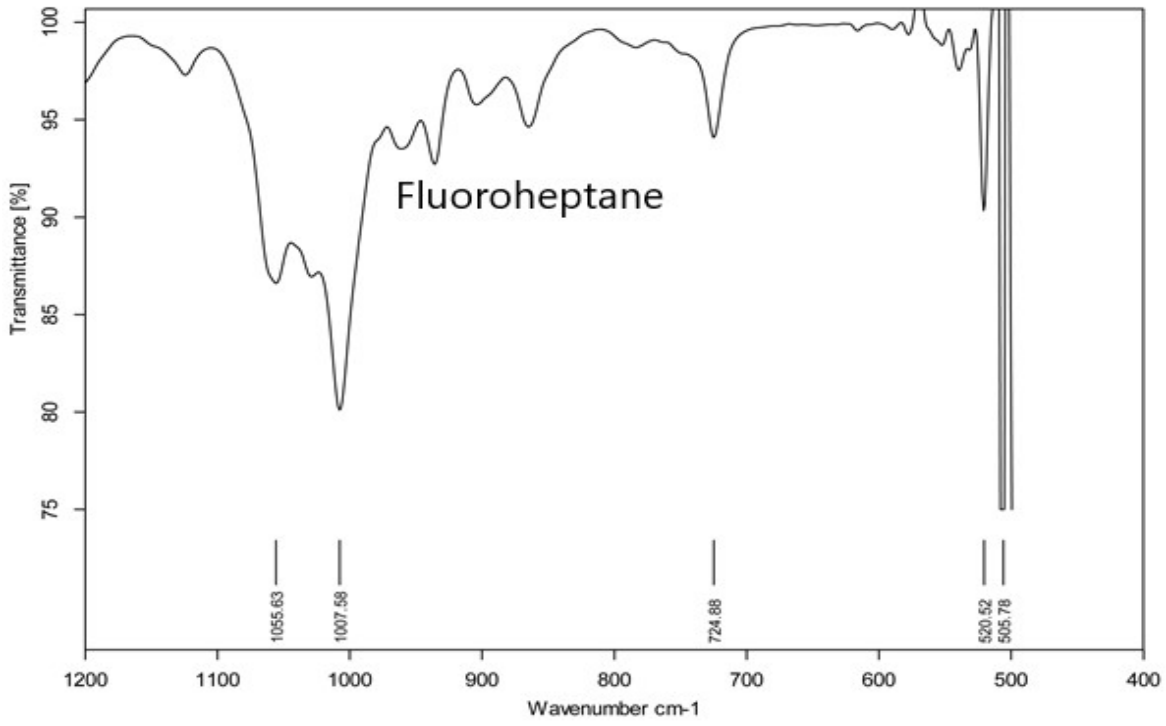
(3) With the experimental wavenumber data, make a graph between wave number *vs.* electronegativity, another between wave number *vs.* Bond length and another wave number bond strength and including in all cases the value of the correlation coefficient.

An example of the results that the students obtained from the experimentation according to the instructions given are shown.

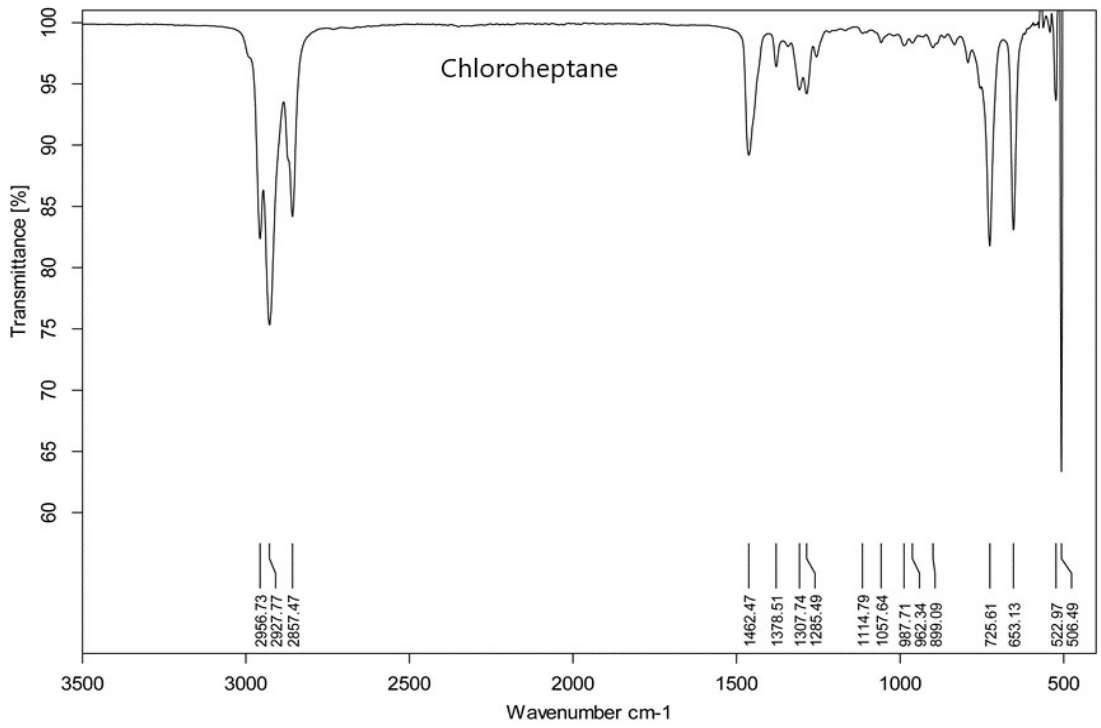
Experimental IR Spectra 1 to 5 were obtained from each of the halo alkanes evaluated in both full and magnification format.



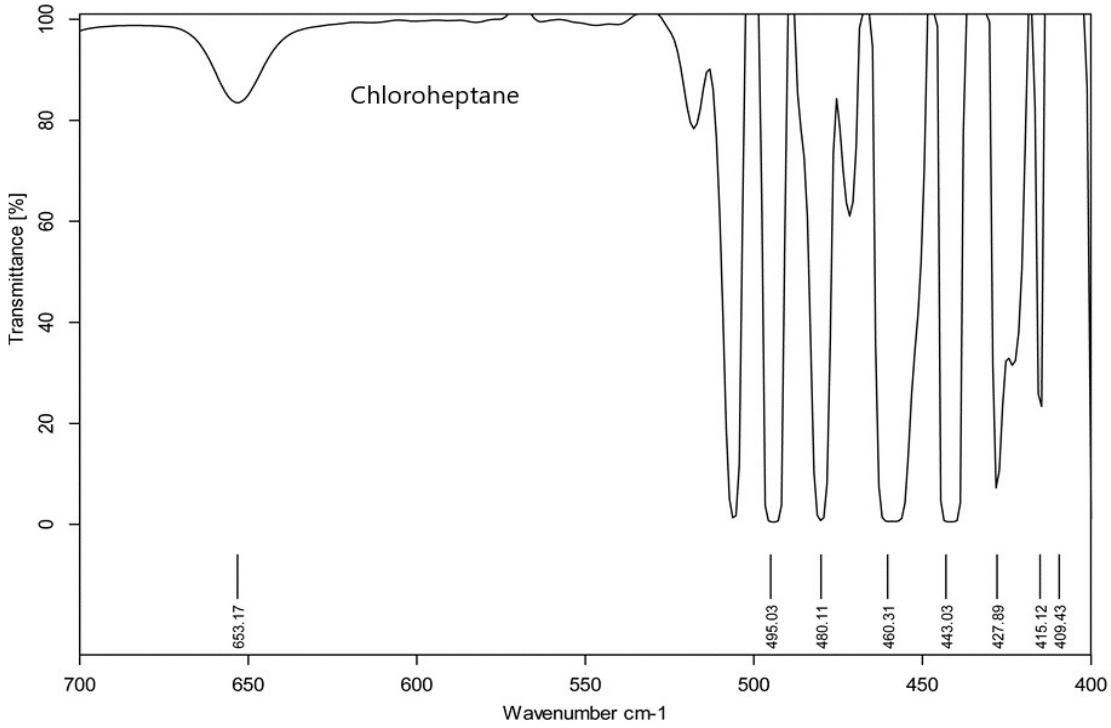
IR Spectra 1A. ATR experimental infrared spectra of 1-Fluoroheptane (400-3500 cm^{-1}) obtained of Bruker Tensor 37 Infrared apparatus



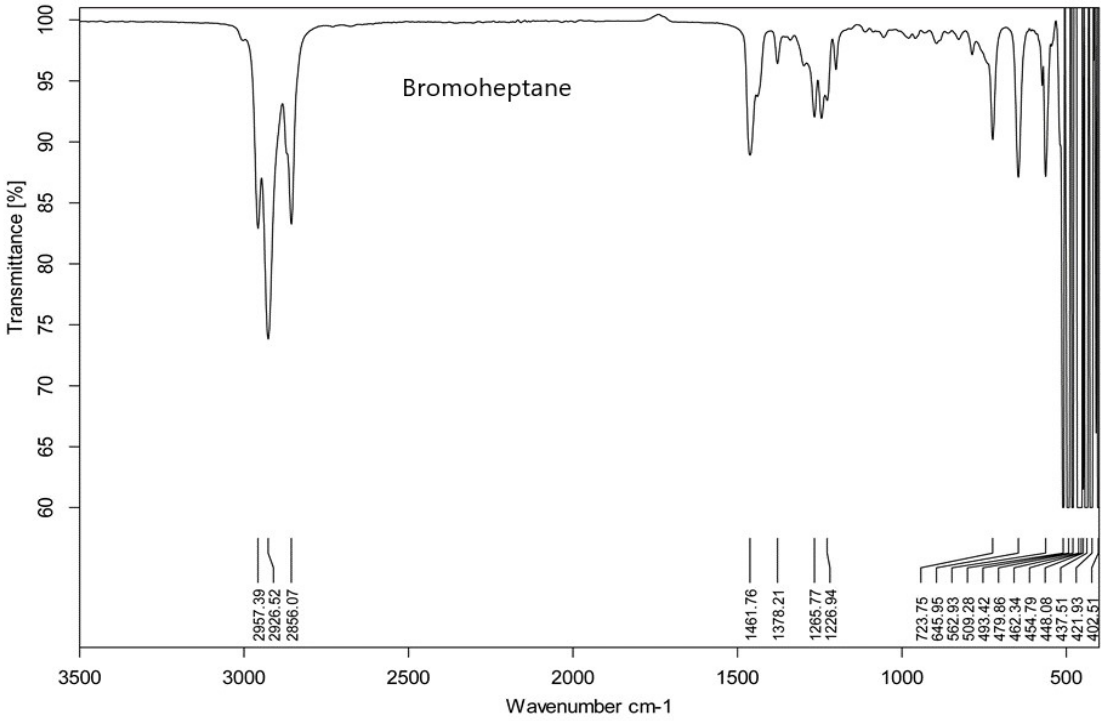
IR Spectra 1B. ATR experimental infrared spectra of 1-Fluoroheptane (1200-400 cm^{-1}) obtained of Bruker Tensor 37 Infrared apparatus



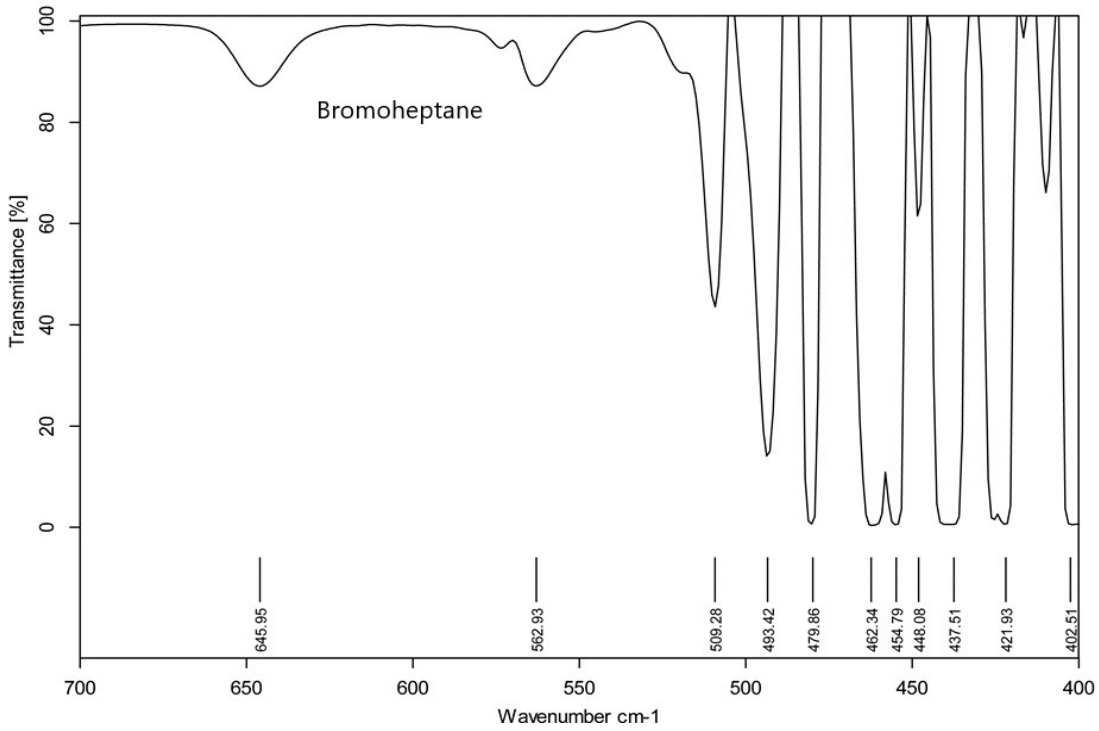
IR Spectra 2A. ATR experimental infrared spectra of 1-Chloroheptane (400-3500 cm^{-1}) obtained of Bruker Tensor 37 Infrared apparatus



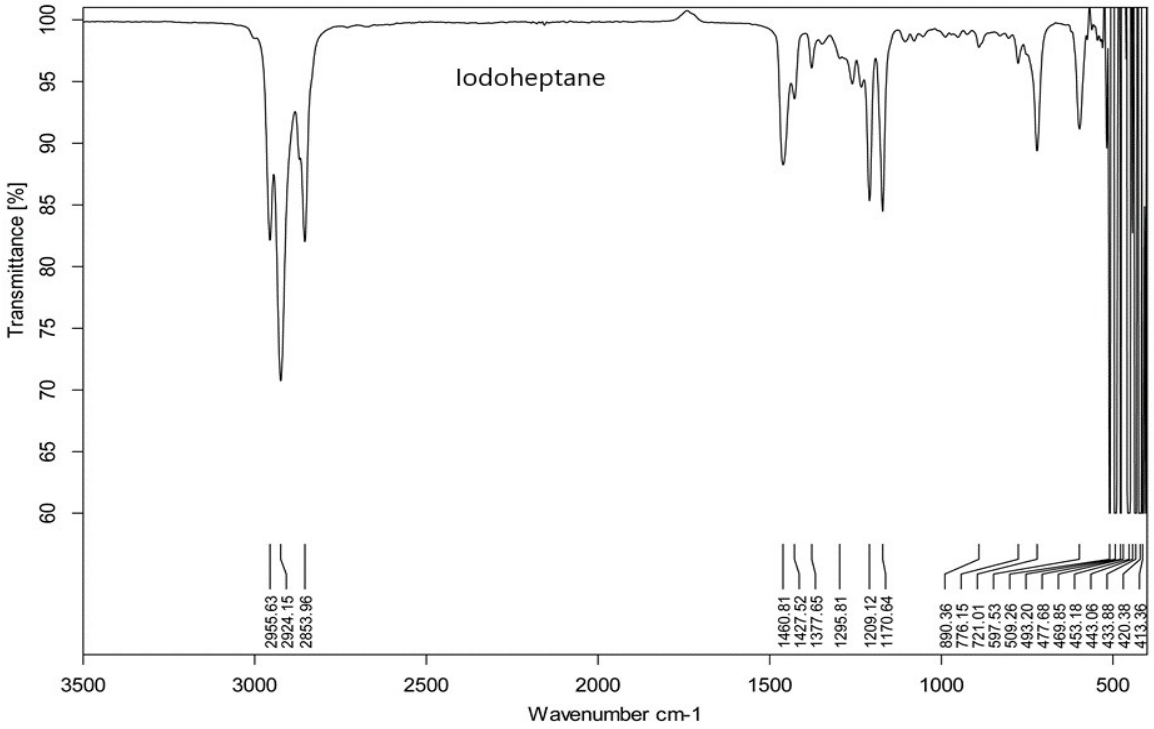
IR Spectra 2B. ATR experimental infrared spectra of 1-Chloroheptane (400-700 cm^{-1}) obtained of Bruker Tensor 37 Infrared apparatus



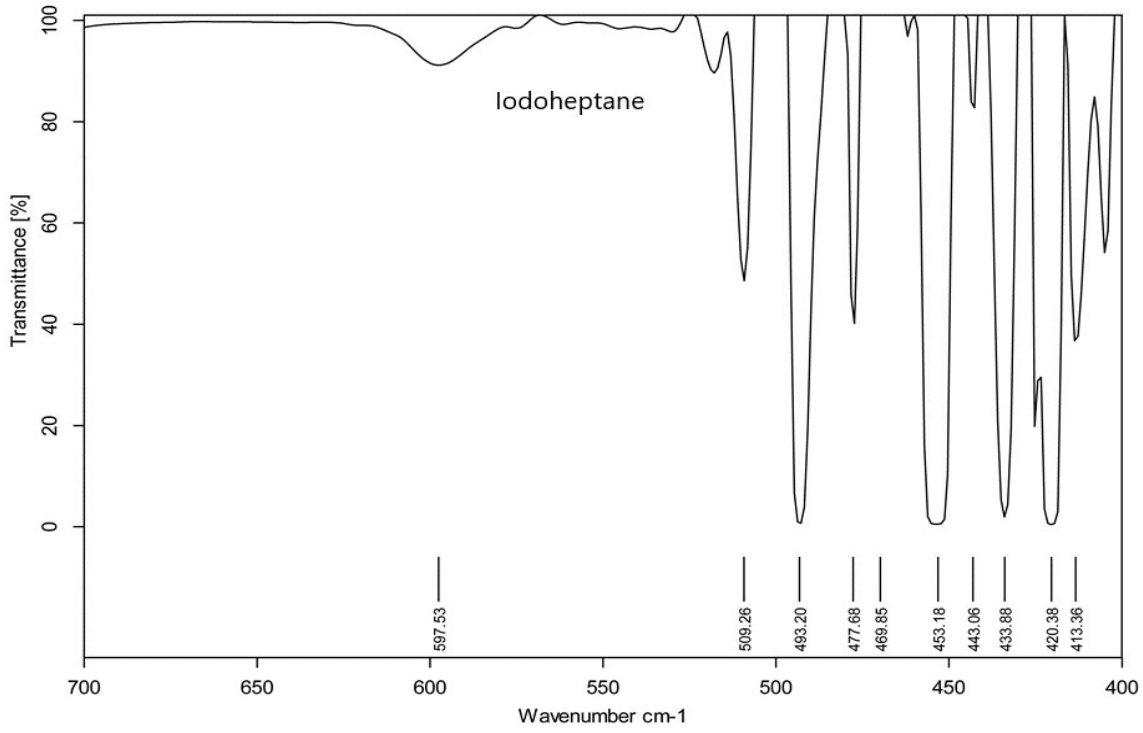
IR Spectra 3A. ATR experimental infrared spectra of 1-Bromoheptane (3500-400 cm^{-1}) obtained of Bruker Tensor 37 Infrared apparatus



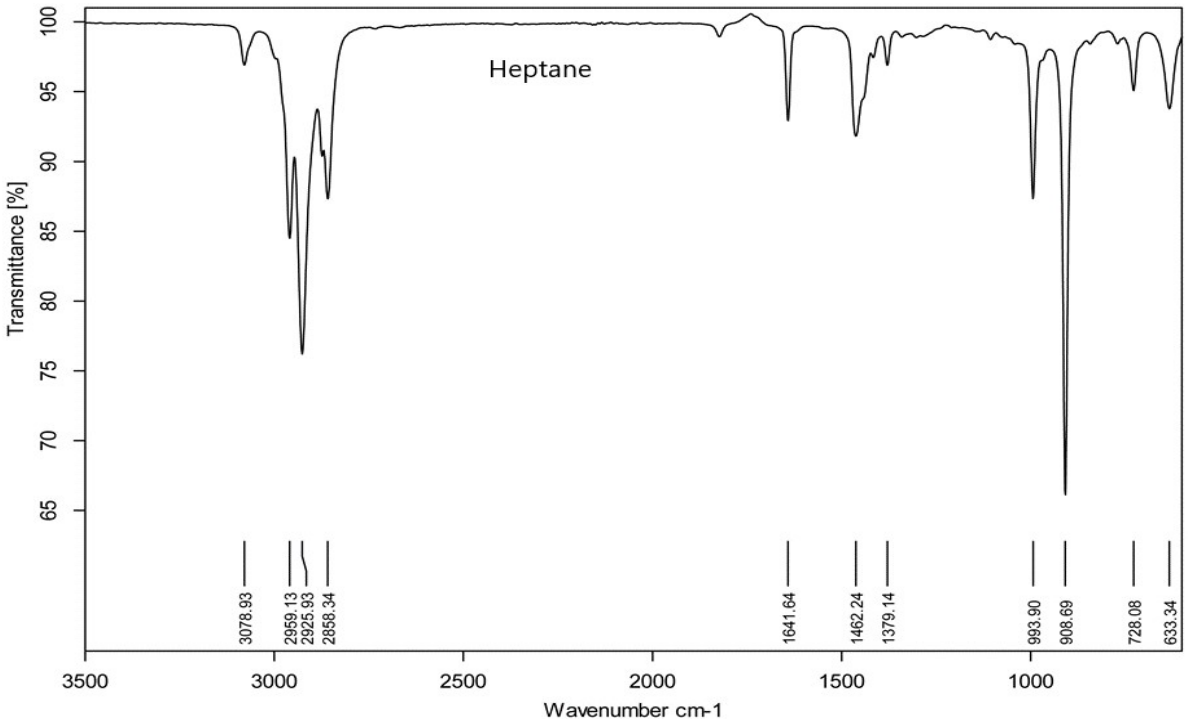
IR Spectra 3B. ATR experimental infrared spectra of 1-Bromoheptane (400-700 cm^{-1}) obtained of Bruker Tensor 37 Infrared apparatus



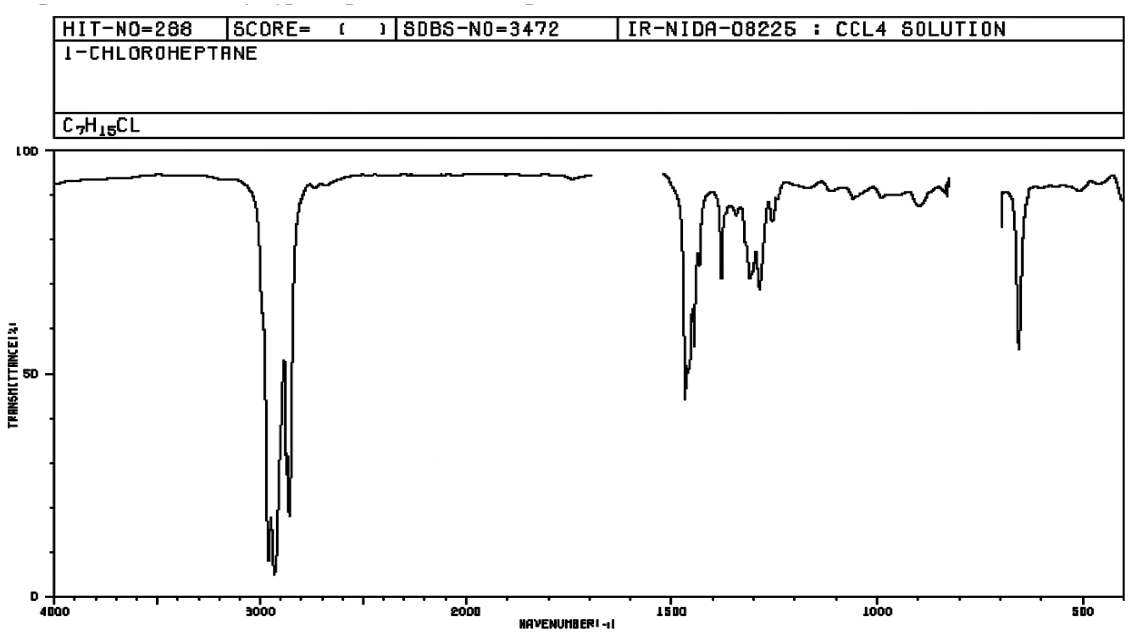
IR Spectra 4A. ATR experimental infrared spectra of 1-Iodoheptane (400-3500 cm^{-1}) obtained of Bruker Tensor 37 Infrared apparatus



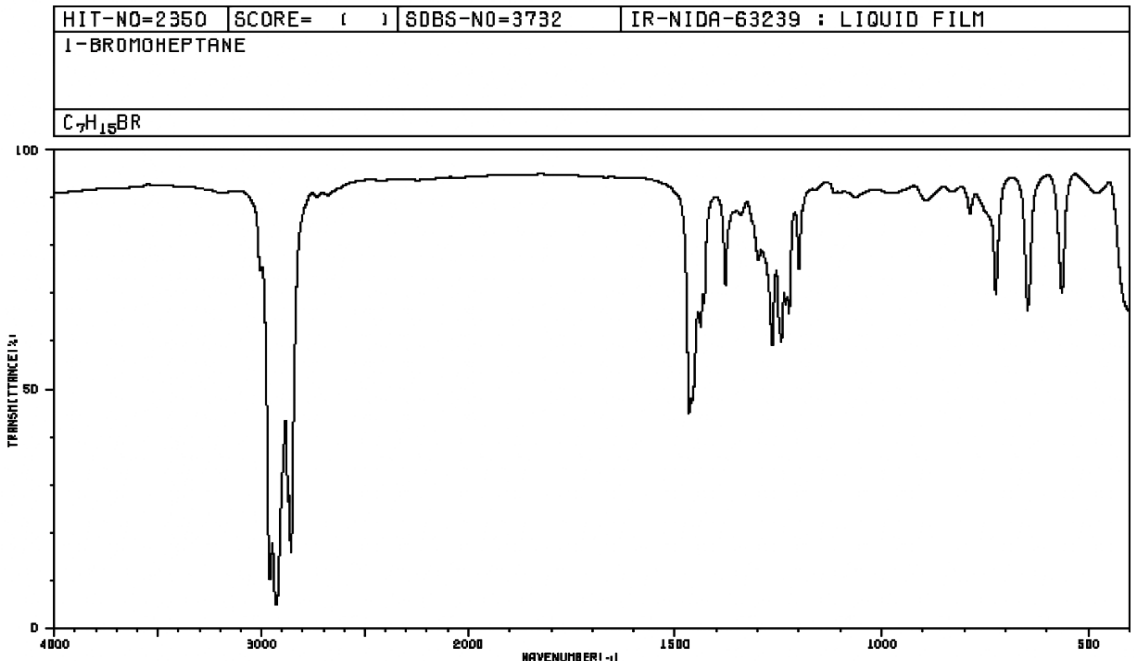
IR Spectra 4B. ATR experimental infrared spectra of 1-Iodoheptane (400-700 cm^{-1}) obtained of Bruker Tensor 37 Infrared apparatus



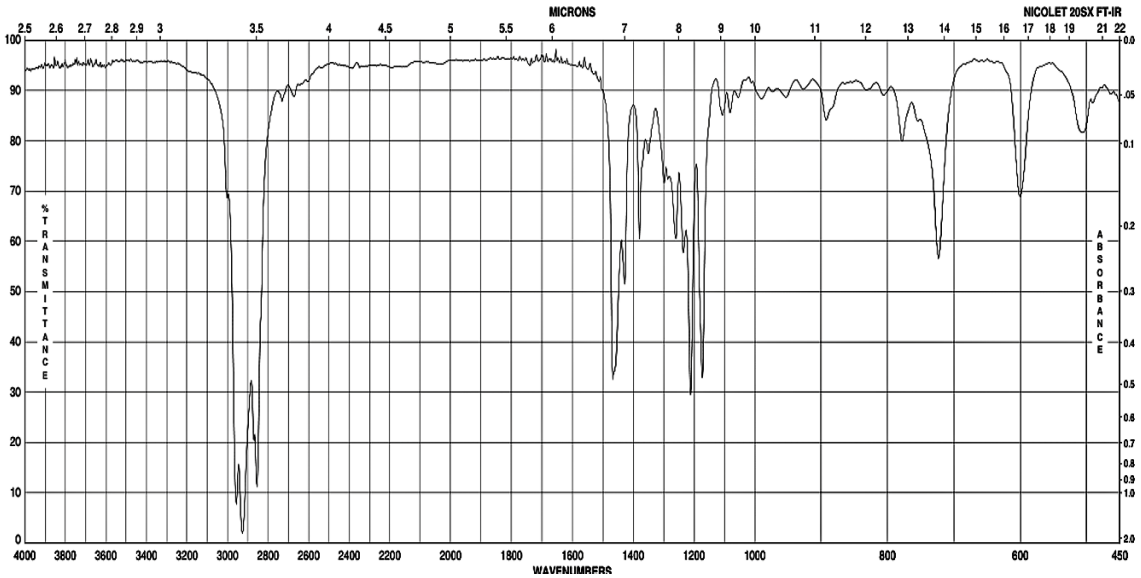
IR Spectra 5. ATR experimental infrared spectra of Heptane (400-3500 cm^{-1}) obtained of Bruker Tensor 37 Infrared apparatus



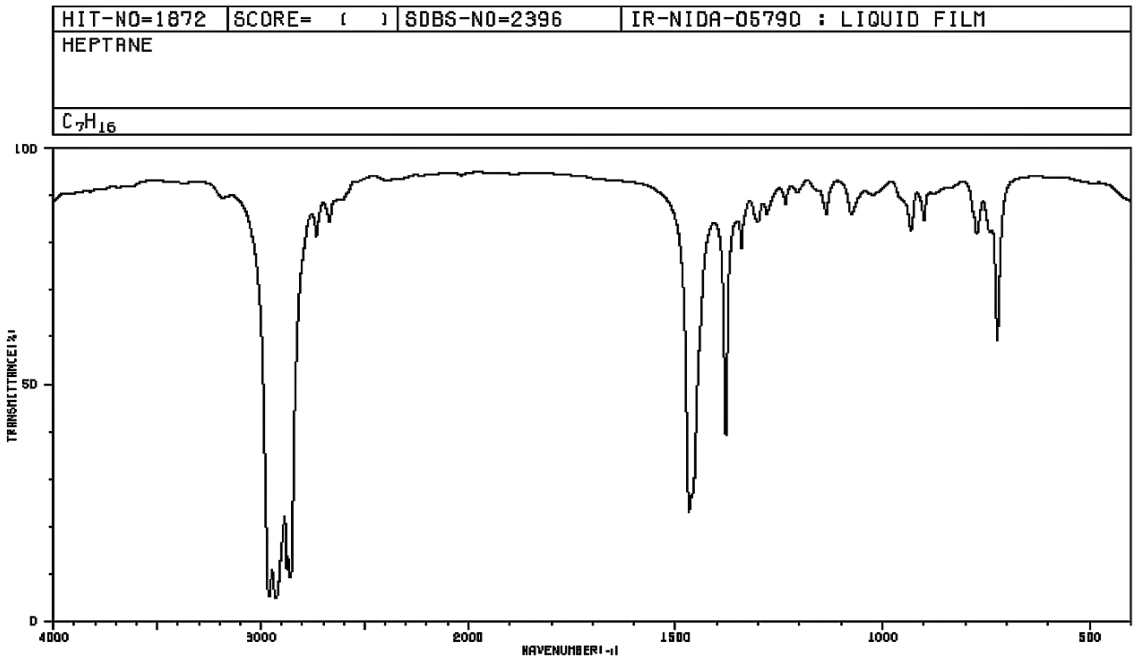
IR Spectra 6. Infrared spectra of 1-Chloroheptane obtained of https://sdbs.db.aist.go.jp/IrSpectralView.aspx?fname=NIDA8225&sdbsno=3472



IR Spectra 7. Infrared spectra of 1-Bromoheptane obtained of https://sdbs.db.aist.go.jp/IrSpectralView.aspx?fname=NIDA8341&sdbsno=3732



IR Spectra 8. Infrared spectra of Iodoheptane obtained of https://www.chemicalbook.com/SpectrumEN_4282-40-0_ESR.htm



IR Spectra 9. Infrared spectra of Heptane obtained from https://sdbs.db.aist.go.jp/IrSpectralView.aspx?fname=NIDA5790&sdbsno=2396

Table 3. Theoretical data of halo alkanes

Bond	**Electronegativity***	**Bond strengths** (kcal/mol)*	**Bond length (Å)***
Carbon-Fluorine	**3.98**	**136**	**0.9170**
Carbon-Chloride	**3.16**	**103**	**1.2746**
Carbon-Bromine	**2.96**	**87**	**1.4145**
Carbon-Iodine	**2.33**	**71**	**1.6090**

Note. * Organic Chemistry, Leroy G. Wade, Jan William Simek, 10th Edition, Global Edition 2022.

In accordance to intructions showed in the procedure previously described and which were shown to the students, as follow we show the corresponding graps making by the students, using the experimental data of the vibration value of streaching C-X bond in cm^{-1}, and the theoretical data of Electronegativity, Bond strengths and Bond length as corresponding. In the plotting are included the r^2 associated to the correlation between both evaluated parameter is shown.

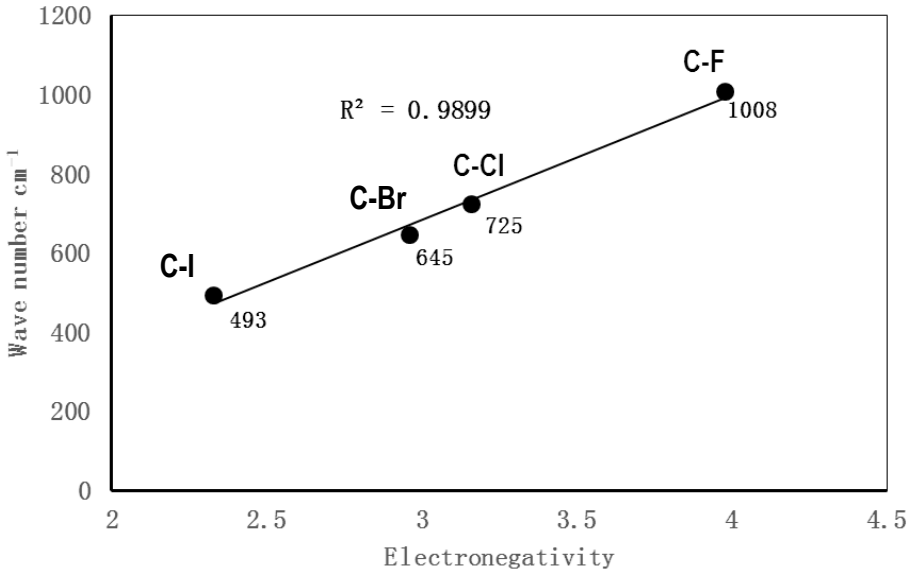


Figure 2. Plotting correlation Electronegativity *vs* Wave number

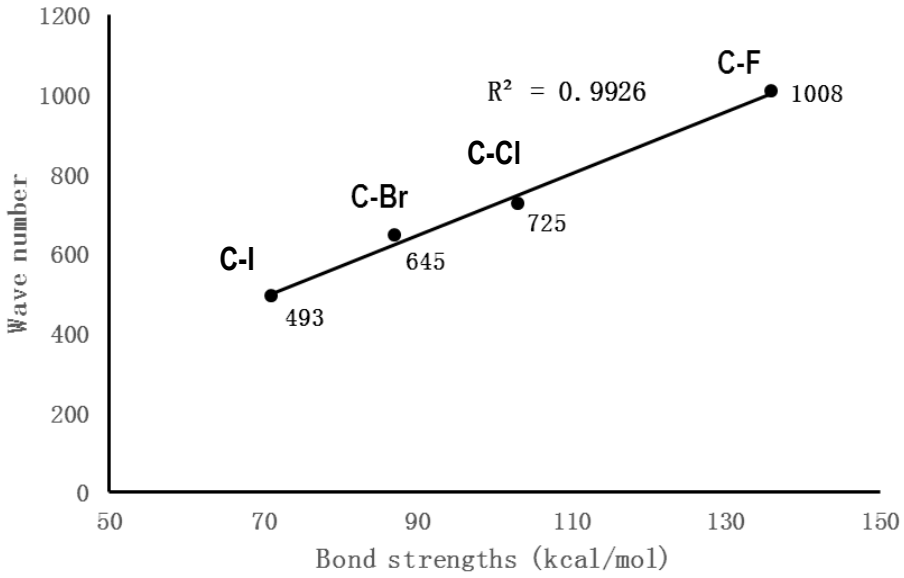


Figure 3. Plotting correlation Wave number *vs* Bond strengths

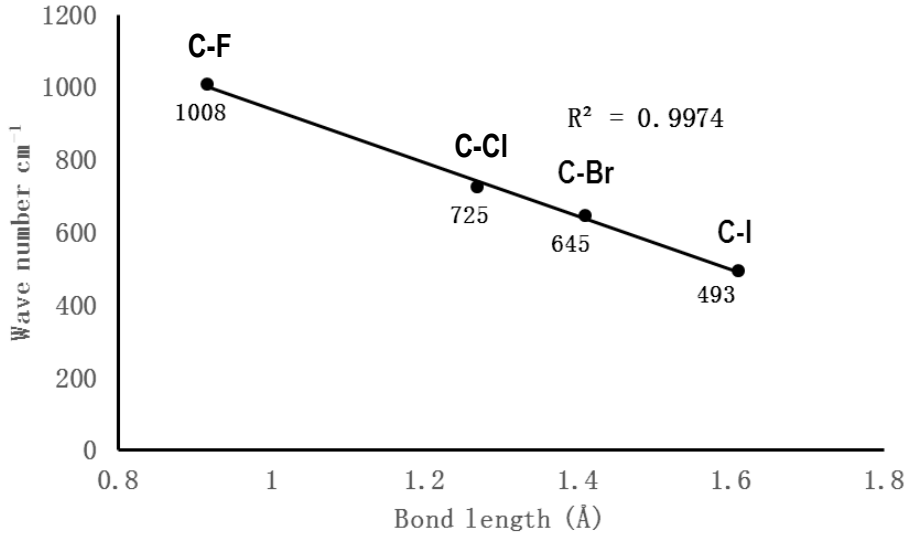


Figure 4. Plotting correlation Wave number *vs* Bond length

5. Discussion

The students who participated in the evaluation were asked to identify the bands of the C-Halogen vibration, as well as the graph where they integrated the value of the wavenumber of each halo alkane *vs.* the value of the theoretical electronegativity reported in tables of the literature. So that they could establish through linear regression, if there is a correlation between the value of electronegativity and the wavenumber observed in the spectrum and how this correlation was. A similar analysis was requested to assess whether there is a correlation between the wavenumber and the bond distance, as well as to assess whether there is a correlation between the wavenumber and the strength of the bond.

This in order for the student to analyze and conclude, if this correlation exists and how large the value of r^2 was used which is the coefficient of determination. In all cases, the students reported correlations greater than 0.98 % and conclude that there is a correlation between electronegativity and the value of the wave number of the C-Halogen stretching vibration that is observed in the infrared spectrum. A similar correlation was observed between the distance of this bond and the wave number where the students obtained correlations greater than 99%, as well as the latter with the energy of the bond that were also greater than 99%.

6. Conclusions

A didactic strategy was developed, for teaching at the undergraduate level to determine the effect that electronegativity has on the vibration response of the C-Halogen bond in a molecule, through a practical experience that involved on the one hand the technique of infrared spectrophotometry and organic molecules with the presence of halogen atoms.

The students indicated that the higher the electronegativity the greater the value of the observed wave number, that the lower the wave number the greater the distance and that the higher the

wave number the binding energy was greater. This allowed them to conclude that due to the strength and distance of the bond between halogen and carbon, the value of the wavenumber is modified, so that, in shorter bonds, greater energy is required for it to vibrate, and in longer and weaker bonds, as in the case of iodine, they vibrate at a lower wavenumber. This allowed students to understand the dependence of electronegativity, bond length, and bond strength over the value observed of the wavenumber detected in an infrared spectrum.

Finally, this study performed in a at higher education level, constitutes a significant contribution to understand the electronegativity effect, the strength and bond distance of the bond stretching between halogen-carbon present in a halo alkane structure using infrared spectroscopically data.

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Authors Contributions

All authors read and approved the final manuscript, the authors contributed as follows: Dr. Adolfo E. Obaya was responsible to validation, methodology, data curation review original draft, supervision and conceptualization; MC Carlos Montaño-Osorio was responsible to writing and editing; QI Vinniza Martínez-Fuentes was responsible to validation, methodology, and data curation; Dr. Benjamin Velasco-Bejarano was responsible to review, editing, formal analysis, review original draft, supervision, funding acquisition, conceptualization.

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Competing Interests

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Informed Consent

Obtained.

Ethics Approval

The Publication Ethics Committee of the Macrothink Institute.

The journal's policies adhere to the Core Practices established by the Committee on Publication Ethics (COPE).

Provenance and Peer Review

Not commissioned; externally double-blind peer reviewed.

Data Availability Statement

The data that support the findings of this study are available on request from the corresponding author. The data are not publicly available due to privacy or ethical restrictions.

Data Sharing Statement

No additional data are available.