CHEMICAL IDENTIFICATION BASED ON SPECTROGRAM

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This thesis is submitted as partial fulfillment of
the requirement for the award of the
Degree in Bachelor of Electrical and Electronics Engineering with Honours

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"I hereby declare that this thesis entitled 'Chemical Identification Based on Spectrogram' is prepared with my own effort unless otherwise stated in any part of this thesis"

Student : ……..

ADEEBAH BINTI JAMAR

Date : ……..……..

Supervisor : ……..…….

DR SUNARDI

Special Dedication To

My Beloved Father
Jamar Bin Sallehudin

My Beloved Mother
Rahmah binti Abdul Manan

My brothers and sister

My Supervisor and Lecturers

All My Friends
For support, love and understanding
During the completion of my degree study

ACKNOWLEDGEMENT

بسم الله الرحمن الرحيم

In the name of Allah, the Most Gracious, the Most Merciful

Alhamdulillah in the name of Allah, first and foremost, I would like to show my gratitude to The Almighty Allah S.W.T for the endless blessings after blessings and giving me the strength and good health to complete this Bachelor's project for the student of degree in Bachelor of Engineering (Electronics) With Honors.

I have finally completed this project successfully. I would like to express my eternal gratitude and appreciate to my supervisor Dr Sunardi for his precious guidance, intuitive comments and suggestions in completing this project. In order to undergo this final year project, there are a number of people that really help me a lot, starting from beginning of the project till the end of it. Without their help, full support and their contribution towards this project, I believe that this thesis will be produced in such a wonderful way.

I wish to express my thankfulness to my family for their support and blessing since the beginning. I also wish to express my appreciation and my deepest gratitude goes to all the technicians and lab assistance. Without their help, this project will never be completed so successful. For those whose name could not be mentioned here one by one, it is a great pleasure to express my gratitude towards all of them.

My most grateful and respect to my father, my mother, my brothers and sisters and all my friends who are the person in my mind that make me pass through all the hard situation throughout the completion of this project. Finally, I would like to thank everyone that has been involved in this project directly or indirectly for their help and contribution.

ABSTRACT

Every chemical has its own element or composition. To determine the presence of this element, spectroscopic technique is used. Spectroscopic technique is a study interaction between matter/chemical with electromagnetic radiation (emr). Each chemical compound will have difference absorbance emr spectrum. In this project, the focus will be on Infrared region. In Infrared region, the functional group presence will be found. Chemical sample that have been use is polyethylene. Polyethylene will be undergoing degradation process with Manganese Laureate. Yield solution of the process will analyze by FTIR and the image of spectrogram will be recorded. In field of Electrical and Electronics Engineering field, the presence of functional group is determined based on image of spectrogram. As conclusion, hope this project will give impact to chemist to make analysis of chemical.

ABSTRAK

Setiap bahan kimia mempunyai unsur atau komposisi tersendiri. Cara untuk mengetahui kehadiran unsur ini di dalam sesuatu bahan kimia dengan menggunakan teknik spektroskopik. Cara ini merupakan kajian interaksi antara radiasi electromagnet dengan bahan kimia. Setiap bahan kima mempunyai kesan serapan di frekuensi yang berbeza di dalam spectrum radiasi electromagnet. Di dalam projek ini kita menumpukan kepada kawasan serapan infra-merah. Di dalam kawsaan ini, kita dapat mengetahui kumpulan befungsi hadir di dalam bahan kimia. Bahan yang digunakan ialah polietilena. Polietilena akan dioksidakan bersama larutan manganese. Dengan menggunakan FTIR, gambar spektrogram akan dirakam. Melalui pendekatan bidang elektrikal dan elektronik, kita akan mengenalpasti kehadiaran kumpulan berfungsi berdasarkan gambar spektrogram yang dirakam. Diharap projek ini dapat membantu ahli kimia untuk menganalisis bahan kimia.

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HDPE	-	High Density Polyethylene
FTIR	-	Fourier Transform Infrared
OH	-	Hydroxyl
CO	-	Carboxyl
C=O	-	Carbonyl

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CHAPTER 1

INTRODUCTION

1.1 Overview

Analytical Chemistry is one of the major branches of modern chemistry. It is subdivided into two main areas, qualitative and quantitative analysis. The former involves the determination of unknown constituents of a substance, and the latter concerns the determination of the relative amounts of such constituents.

In the field of Electrical and Electronic Engineering, we want try to develop system for chemical analysis based on spectrogram. A spectrum can be used to obtain information about atomic and molecular energy levels, molecular geometries, chemical bonds, interactions of molecules, and related processes [1]. Often, spectra are used to identify the components of a sample (qualitative analysis). Spectra may also be used to measure the amount of material in a sample (quantitative analysis).This project will use image of spectrogram to make an analysis for chemical easily.

Spectroscopy, or the study of the interactions of electromagnetic radiation (emr) with matter, is the largest and most nearly accurate class of instrumental methods used in chemical analysis and indeed in all of chemistry. The electromagnetic spectrum is divided into the following wavelength regions: gamma-ray, X-ray, ultraviolet, visible, infrared, microwave, and radio. The interactions of emr with matter involve absorption or emission of emr energy. The matter-emr interactions take place in devices called spectrometers, spectrophotometers, or spectroscopes. The spectra produced in these devices may be recorded graphically or photographically in images called spectrograms, which permit convenient study of the wavelengths and intensities of the emr absorbed or emitted by the sample being analysed.

1.1 Problem Statement

Some basic properties of the sample can be determined by the wavelengths and amount of light absorbed or the radiant energy emitted by sample into a wave spectrum. A given sample will not absorb all wavelengths equally. Because different samples absorb light at different wavelengths, a spectrometer can be used to distinguish compounds by analysing the pattern of wavelengths absorbed by a given sample. The result will record as spectrogram.

From the spectrogram, chemist needs to analyse each spectrogram to check any possible of abnormality. The abnormality of the spectrogram between each other will contribute to different analysis.

This project will help chemist to identify the abnormality of spectrogram to come out with better analysis and result.

1.2 Project Description

In chemical field, to analysis chemical sample, one of method is based on spectrogram. The spectrogram is generated from software of FTIR as an image. To analysis data of spectrogram as in image format is not relevant.

To solve this problem, the image of spectrogram will be converting into a signal. The main part of this project is to develop system for converting image of spectrogram into signal. The signal will have same characteristic as spectrogram. The presence of peak in signal will help to obtain information about chemical bonding and functional group.

1.3 Objective

The objective of this project is to identify the functional group of HDPE based on wavelength from spectrogram

1.4 Project Scope

To accomplish this project in order to work successfully, there are a few things to define in the scopes of the project. There are:

i) The chemical sample is High Density Polyethylene, HDPE and 1% Manganese laureate.
ii) Interpretation of HDPE
iii) Interpretation presence of Manganese in HDPE
iv) Interpretation of Functional Group after degradation of HDPE

CHAPTER 2

LITERATURE REVIEW

2.1 Electromagnetic Radiation (EMR)

Light travels through space in the form of radiant energy [2]. Electromagnetic radiation can be arranged according to their wavelengths and frequencies called Electromagnetic Spectrum. It divided to following wavelength regions gamma-ray, X-ray, ultraviolet, visible, infrared, microwave, and radio as Figure 2.1.

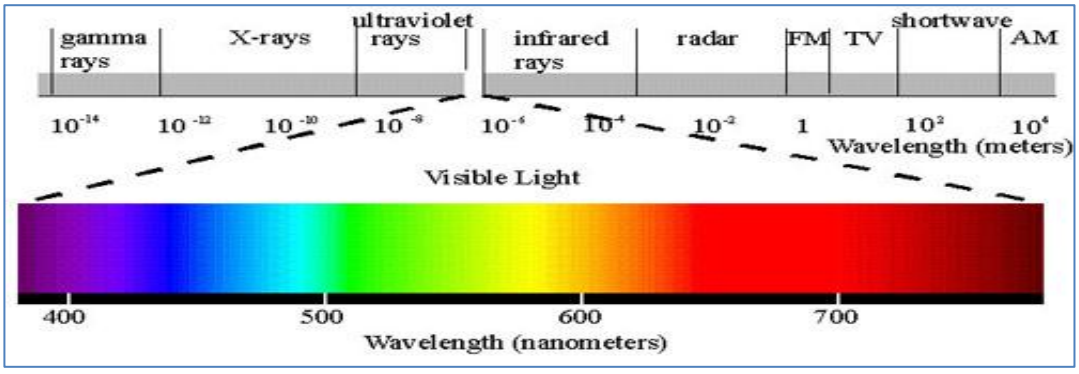


Figure 2.1 Electromagnetic Spectrum

2.2 Polyethylene

Before considering the interpretation of the spectrum of polyethylene, it is necessary to know the structure of the molecule. Although polyethylene may be considered to a first approximation as an infinite chain of CH_2 groups, the chains are found in essentially two different configurations [3]. In the crystalline regions, whose structure is known from x-ray diffraction studies, 2 the chain is found in the planar zig-zag configuration. In the amorphous regions, which can constitute up to half of the specimen, the chain configuration is an essentially random one restricted only by the conservation of bond angles and distances. The random figuration in the amorphous regions becomes a partially oriented one when the sample is stretched. It is thus very important to keep in mind that the usual spectrum of polyethylene represents a superposition of the spectra of two different types of chain configurations. The spectra of these two components are not identical, and failure to recognize this has led to erroneous assignments

2.3 Hydrogen Bonding

The presence of hydrogen bonding is of great importance in a range of molecules. Hydrogen bonding is defined as the attraction that occurs between highly electronegative atoms carrying a non-bonded electron pair [3]. Hydrogen atom itself bonded to a small highly electronegative atom. The example of this type of bonding as illustrated in Figure 2.2. It calls intermolecular hydrogen bonding. Hydrogen bonding is very important. This bonding influences the bond stiffness and so alters the frequency of vibration.

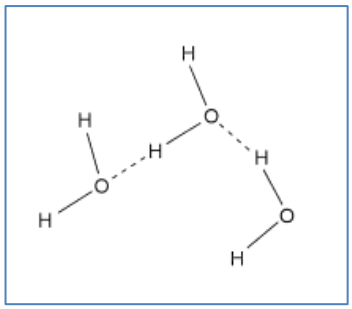


Figure 2.2: Hydrogen bonding in H_2O

2.4 Spectrometers

Late 1940, chemical identification or testing was done by selective separations and absolute determinations all based on gravimetric and volumetric techniques. It now referred to as classical chemical analysis. These classical methods require high analytical skill and are very accurate in the hands of skilled operators. Sadly this method is also very slow and cannot be readily adapted for the rapid analysis of large numbers of samples.

Spectroscopy is an analytical technique which helps determine structure. The amount of light absorbed by the sample is measured as wavelength is varied. Spectrometer is an instrument that measures the fraction of the incident light transmitted [4] through a solution. In other words, it is used to measure the amount of light that passes through a sample.

Spectrometers spread light out into wavelengths called "spectra," which look something like rainbow-colored bars. Using the spectra, scientists can look for and study the "emission lines" and "absorption lines" that are sort of fingerprints of atoms and molecules that may be present as Figure 2.3. Each atom has a unique fingerprint [2] because each can only emit or absorb certain wavelengths of energy. Thus, the fingerprint -- as seen in the location and spacing of spectral lines -- is unique for each atom.

Figure 2.3 Emission and Absorption lines as "fingerprints"

A given compound will not absorb all wavelengths equally [5]. That why some compounds absorb only wavelengths outside of the visible light spectrum, and that's why there are colorless solutions like water. Because different compounds absorb light at different wavelengths, a spectrometer can be used to distinguish compounds by analysing the pattern of wavelengths absorbed by a given sample.

2.5 Spectroscopic Techniques

The spectroscopic techniques described below do not provide a three-dimensional picture of a molecule, but instead yield information about certain characteristic features. A brief summary of Infrared Spectroscopy

•**Infrared Spectroscopy**:

Absorption of this lower energy radiation causes vibrational and rotational excitation of groups of atoms within the molecule. Because of their characteristic absorptions identification of functional groups is easily accomplished.

2.6 Theory Absorption of Infrared Region

At temperatures above absolute zero, all the atoms in molecules are in continuous vibration with respect to each other. When the frequency of a specific vibration is equal to the frequency of the IR radiation directed on the molecule, the molecule absorbs the radiation [5].

The major types of molecular vibrations are stretching and bending. The various types of vibrations are illustrated in Figure 2.3(a) and Figure 2.3(b). Infrared radiation is absorbed and the associated energy is converted into these types of motions. The absorption involves discrete, quantized energy levels [5]. However, the individual vibrational motion is usually accompanied by other rotational motions. These combinations lead to the absorption bands, not the discrete lines, commonly observed in the mid IR region.

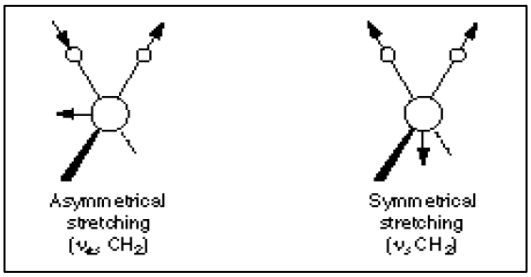


Figure 2.3(a) Stretching Vibration [5]

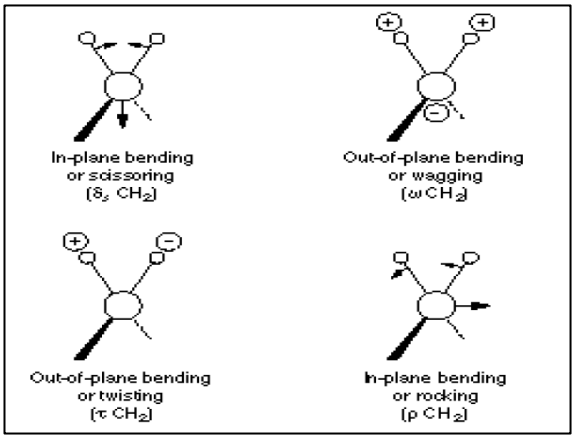


Figure 2.3(b) Bending Vibration [5]

2.7 Spectrum Manipulation: Difference Spectra

The most straightforward method of analysis for complex spectra is difference spectroscopy. This technique may be carried out by simply subtracting the infrared spectrum of one component of the system from the combined spectrum to leave the spectrum of the other component [6]. If the interaction between components result in a change in the spectral properties of either one or both of the component, the changes will be observed in the difference spectra. Such changes may manifest themselves via the appearance of negative and positive peak in spectrum.

Spectra subtraction may be applied to numerous applications can be used for the data collected solution. In order to obtain the spectrum of a solution, it is necessary to record spectra of both the solution and solvent alone. The solvent spectrum may then be subtracted from the solution spectrum.

2.8 Degradation Process

Degradation due to the oxidation process as a result of exposing samples to the hot Manganese solution at 70°C for 1000 hours was detected by FTIR. Increase of the hot Mangnese solution exposure duration led to a significant increase in the carbonyl group concentration due to the higher oxidation of the molecules. The increase in the carbonyl band region (1600–1800 cm^{-1}) is a characteristic for thermal degradation. Carbonyl groups usually account for most of the oxidation products on thermo-oxidative degradation of polyethylene; the concentration of carbonyl groups can be used to monitor the progress of degradation [7]. The carbonyl absorption is composed of different overlapping bands corresponding to acids, ketones , aldehydes and lactones . The growth of carbonyl absorbance was almost negligible for all samples during the hot Manganese solution exposure for 1000 hours. At 1000 hours of exposure, HDPE showed a large increase in carbonyl region. Other bands such as hydroxyl, ester and vinyl group are also present. HDPE show various band presence near 3500–4000 cm^{-1} in the FTIR spectrum. The bands appeared to be due to the large number of terminal –OH groups resulting from the bond scission due to the thermal degradation. The new

band at 1600–1800 cm^{-1} was assigned to the carbonyl stretching vibration from the oxygenated product [8].

2.9 Method to analyse spectra

When do the analysis for the spectra, it is easier to follow a series of steps in examining each spectrum [9].

Step 1:

Look first for the carbonyl C=O band. Look for a strong band at 1820-1660 cm^{-1}. This band is usually the most intense absorption band in a spectrum. It will have a medium width. If there is the carbonyl band, look for other bands associated with functional groups that contain the carbonyl by going to step 2. If no C=O band is present, check for alcohols and go to step 3.

Step 2:

If a C=O is present, then determines if it is part of an acid, an ester, or an aldehyde or ketone.

ACID	Look for indications that an O-H is also present. It has a broad absorption near 3300-2500 cm^{-1}. This actually will overlap the C-H stretch. There will also be a C-O single bond band near 1100-1300 cm^{-1}. Look for the carbonyl band near 1725-1700 cm^{-1}.
ESTER	Look for C-O absorption of medium intensity near 1300-1000 cm^{-1}. There will be no O-H band.
ALDEHYDE	Look for aldehyde type C-H absorption bands. These are two weak absorptions to the right of the C-H stretch near

	2850 cm^{-1} and 2750 cm^{-1} and are caused by the C-H bond that is part of the CHO aldehyde functional group. Look for the carbonyl band around 1740-1720 cm^{-1}.
KETONE	The weak aldehyde CH absorption bands will be absent. Look for the carbonyl CO band around 1725-1705 cm^{-1}.

Step 3:

If no carbonyl band appears in the spectrum, look for an alcohol O-H band.

ALCOHOL	Look for the broad OH band near 3600-3300 cm^{-1} and a C-O absorption band near 1300-1000 cm^{-1}.

Step 4:

If no carbonyl bands and no O-H bands are in the spectrum, check for double bonds, C=C, from an aromatic or an alkene.

ALKENE	Look for weak absorption near 1650 cm^{-1} for double bonds. There will be a CH stretch band near 3000 cm^{-1}.
AROMATIC	Look for the benzene, C::C, double bonds which appear as medium to strong absorptions in the region 1650-1450 cm^{-1}. The CH stretch band is much weaker than in alkenes.

Step 5:

If none of the previous groups can be identified, you may have an alkane.

ALKANE	The main absorption will be the C-H stretch near 3000 cm^{-1}. The spectrum will be simple with another band near 1450 cm^{-1}.

Step 6:

If the spectrum still cannot be assigned you may have an alkyl bromide.

ALKYL BROMIDE	Look for the C-H stretch and a relatively simple spectrum with an absorption to the right of 667 cm^{-1}.

CHAPTER 3

MATERIAL AND METHODE

3.1 Overview

Through this chapter, all the process involved in project will be discussed. Planning of time is the first step has be done upon the development process will be finished before the deadline.

This include the theoretical and technique used in the project. The process of collecting data and software development process such that the frame work would be contributing to the project succeed. Reference a method implies is made where appropriate.

3.2 Hardware Requirements

3.2.1 Fourier Transform Infrared Spectroscopy, FTIR Spectroscopy

Infrared Spectroscopy (IR) is an analytical technique for chemical compound identification. It is based on the fact that different chemical functional groups absorb infrared light at different wavelength dependent upon the nature of particular chemical functional group. A Fourier Transform is a mathematical conversion that allows the split of the entire infrared light spectrum simultaneously, then converting the scanning results mathematically into a wavelength versus absorbance spectra [10].

Combined together these two functions provide Fourier Transform Infrared Spectroscopy as an instrument that can be used in the identification characterization of organic compound [10]. The relative simplicity of the resulting FTIR analytical methods allows it to be widely used for the analysis of a wide range of different materials. It is often used in the packaging industry to analyse monomeric materials for purity, and to identify polymers and their composition.

FTIR Spectroscopy that use in this project is from model Thermo Nicolet Avatar 370 as show in Figure 3.1.

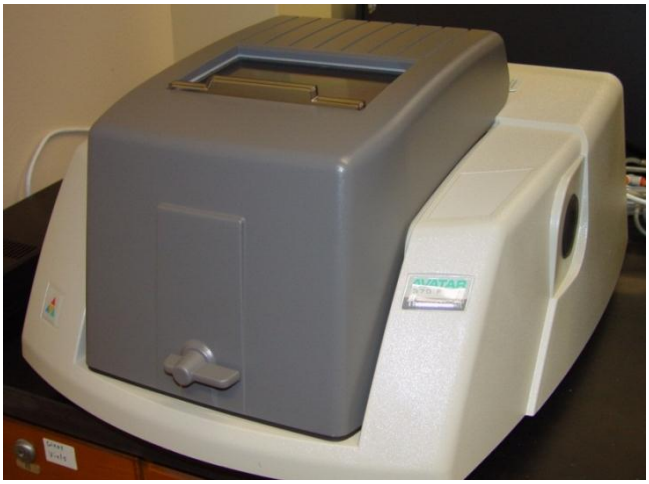


Figure 3.1: FTIR Spectroscopy model Thermo Nicolet Avatar 370

3.2.2 Sample : High Density Polyethylene, HDPE

Sample that introduce in this project is High Density Polyethylene, HDPE. HDPE produce by Faculty of Chemical and Natural Resources Engineering, FKKSA University Malaysia Pahang. The experiment is carried out with HDPE at Biological Laboratory of FKKSA.

It is natural to begin with this polymer since it is structurally the simplest and has a relatively uncomplicated spectrum. High Density Polyethylene (HDPE) ($0.941 \leq$ density <0.965) is thermoplastic material composed of carbon and hydrogen atom joined together forming high molecule weight product such in Figure 3.4 [101. Methane gas as shown in Figure 3.2 is converted into ethylene as in Figure 3.3. Then, with the application of heat and pressure, the ethylene is converted into polyethylene [11].

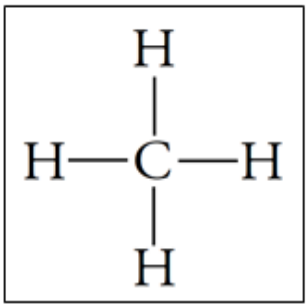


Figure 3.2: Methane

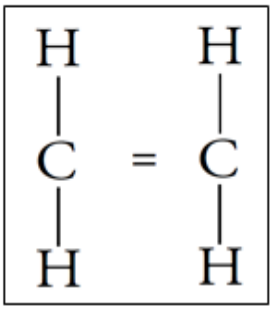


Figure 3.3: ethylene

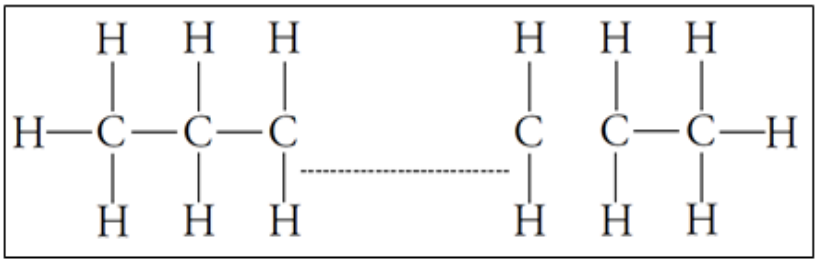


Figure 3.4: Polyethylene Molecular Chain

3.3 Software Requirements

3.3.1 OMNIC from Thermo Scientific

After HDPE undergo analysis with FTIR spectroscopy, the result of the experiment will generate by a software call OMNIC. This software will generate the result as spectrogram. The spectrogram is use as data to be analysing later.

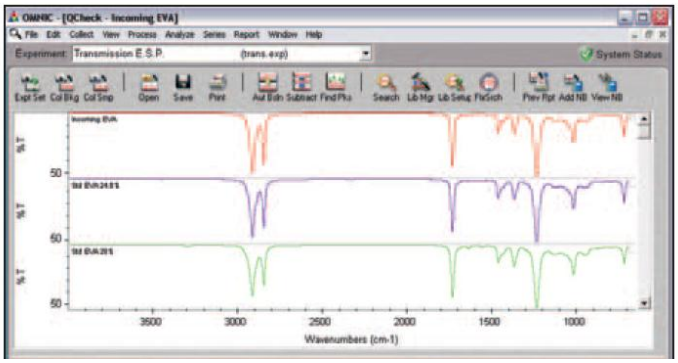


Figure 3.5: OMNIC Software use to generate Spectrogram

3.3.2 Matrix Laboratory, MATLAB

In this project, MATLAB Software used is version R2011b, 32bit. MATLAB is use for develop program for converting the image of Spectrogram into the signal.

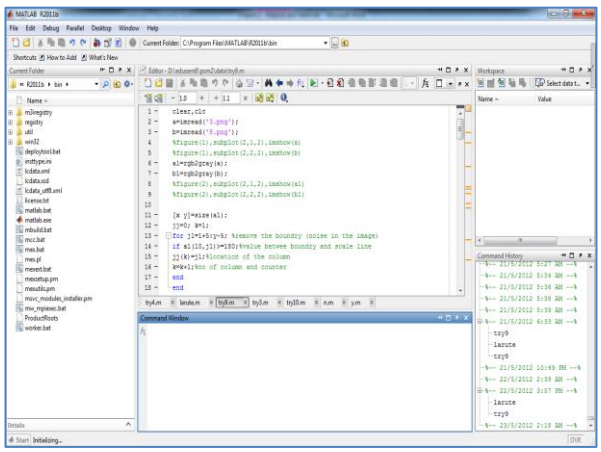
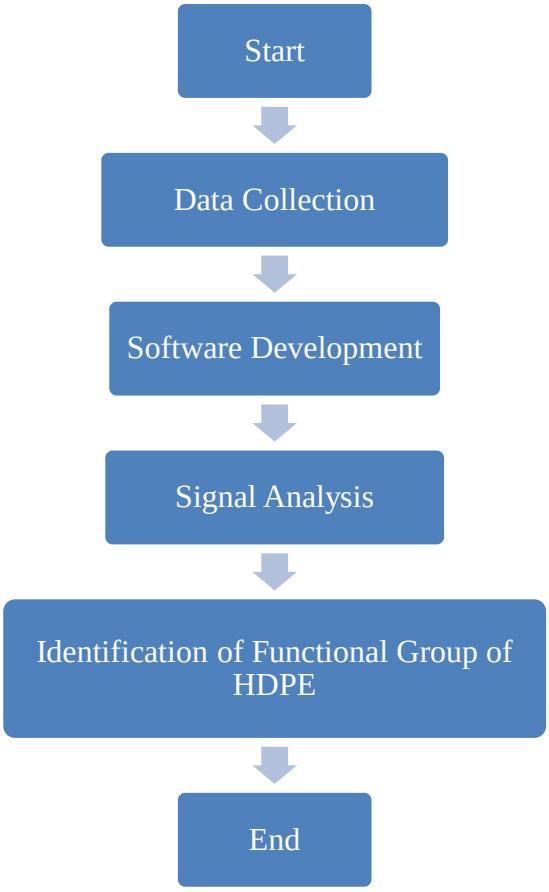


Figure 3.6: MATLAB Software

3.4 Project Development

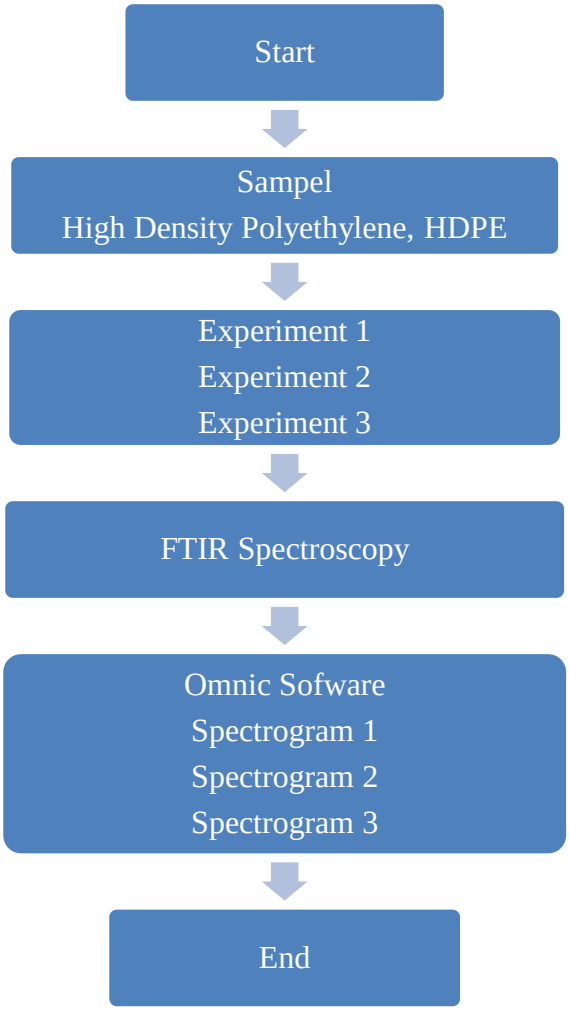
Development process of the overall project is based on following Flow Chart 1.



Flow Chart 3.1: Project Development

3.5 Data Collection

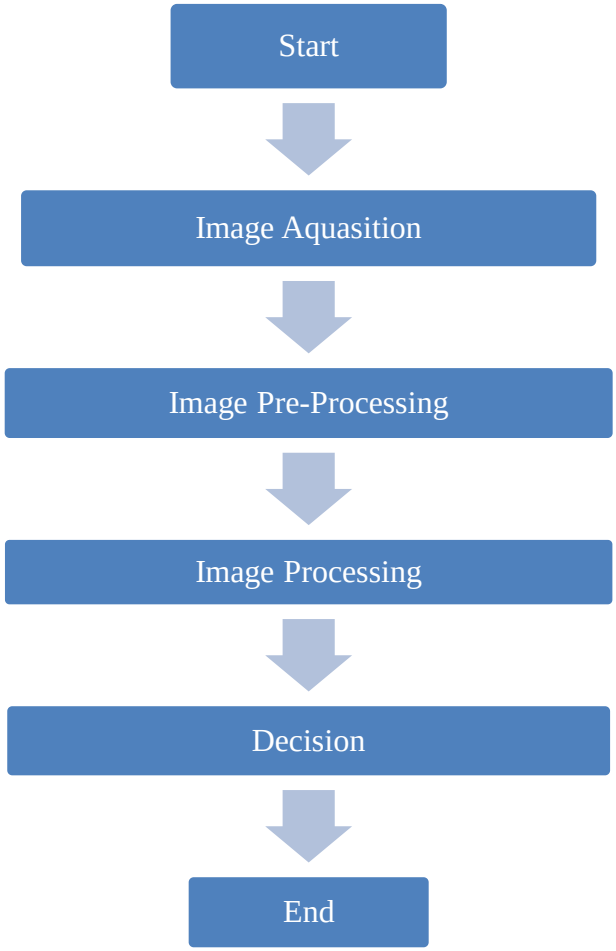
In this project, image of spectrogram is determined as the data. Flow Chart 3.2 shows the process of getting image of spectrogram of High Density Polyethylene, HDPE. The data is collect based on following Flow Chart 3.2.



Flow Chart 3.2: Data Collection

3.6 Software Development

Development process of the software by MATLAB to process the image is based on following Flow Chart 3.2



Flow Chart 3.3: Software Development

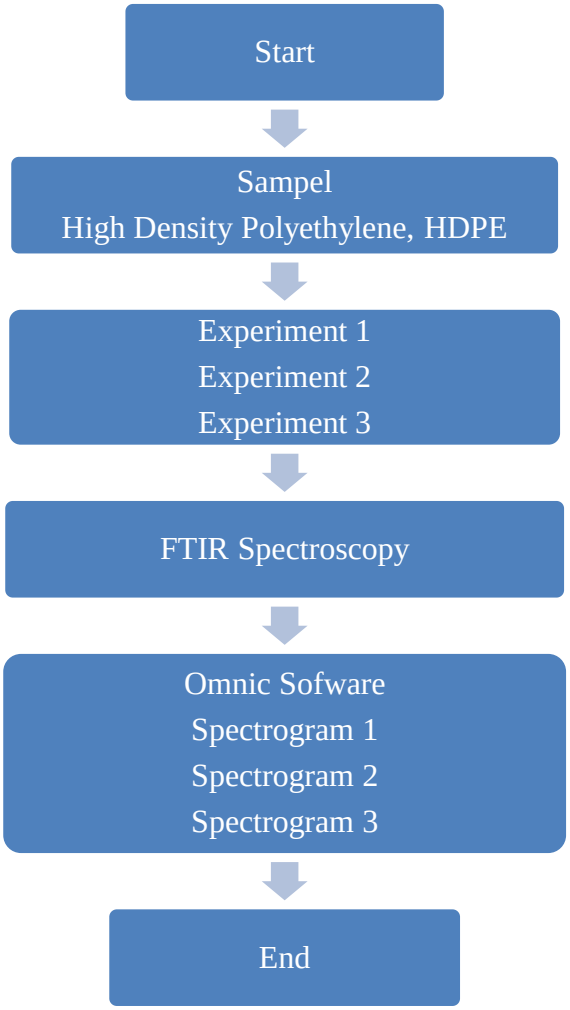
CHAPTER 4

EXPERIMENTAL AND SOFTWARE DEVELOPMENT

4.1 Overview

In this chapter the method of experimental and software development will be discuss with the detail explanation. Part of Experimental will discuss about method for collecting the data. The discussion is about the process about getting spectrogram from chemical compound HDPE. Second part is Software Development. In this part, the process of converting the image of spectrogram into signal will be explained in detail.

4.2 Experimental and Data Collection



Flow Chart of Experimental and Data Collection

There are 3 types of experiments were carried out. Aim to perform of all the experiments is to get the spectrogram. Experiment 1 and 2 is perform to analyse the presence of HDPE and Manganese. Experiment 3 is carried out to determine the presence of functional group of HDPE.

To determine the functional group of HDPE, it must be undergo process of degradation. In this experiment, HDPE is expose to the hot Manganese Carboxylates solution at 70°C for 1000 hours. This process call thermal degradation technologies. Thermal degradation technologies have several techniques which are

pyrolysis,hydrogenation and thermal cracking [12]. Technique of prolysis is choose for this experiment.After undergo the thermal proces, the sample will be analyse by FTIR and generate the spectrogram by the software.

4.2.1 Experiment 1: Interpretation of High Density Polyethylene

Objective:

To classify the presence of High Density Polyethylene, HDPE

Material:

High Density Polyethylene, HDPE

Equipment:

FTIR

Methodology:

Analyse HDPE with FTIR. Generate the Spectrogram of HDPE by using Omnic Software

Result:

Spectrogram of HDPE as show in Figure 4.1

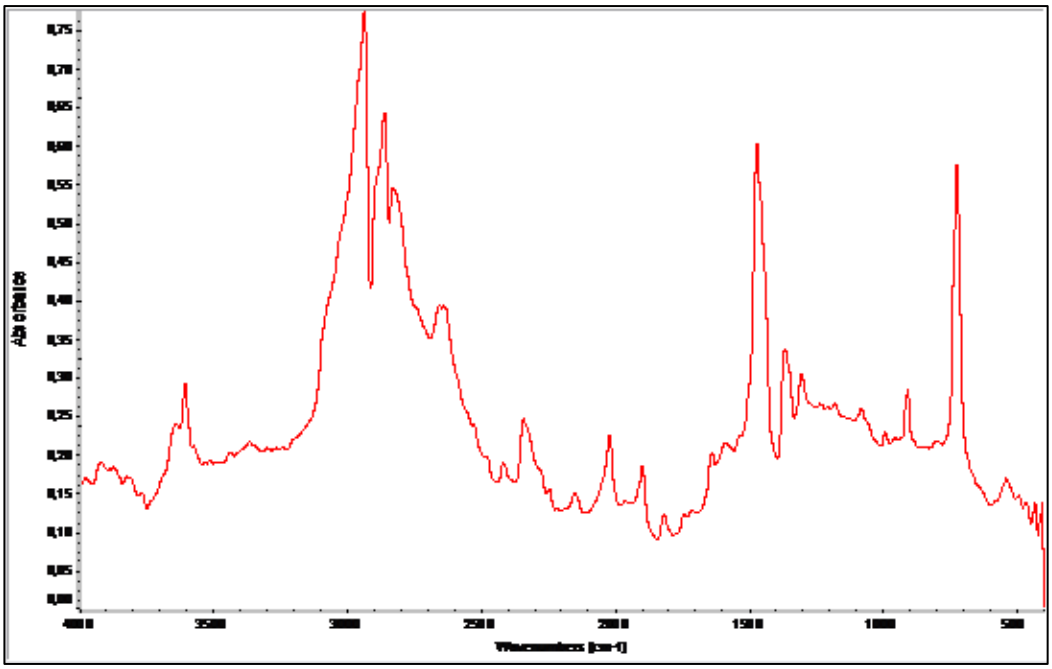


Figure 4.1: Spectrogram of HDE

4.2.2 Experiment 2: Interpreting the presence of 1% Manganese laureate

Objective:

To identify the presence of 1% Manganese laureate in High Density Polyethylene, HDPE

Material:

HDPE and 1% Manganese laureate

Methodology:

1% Manganese laureate is added into HDPE. The solution is analyse by using FTIR. Spectrogram of the solution is generated by Omnic software.

Result:

Spectrogram of the solution is show in Figure 4.2.

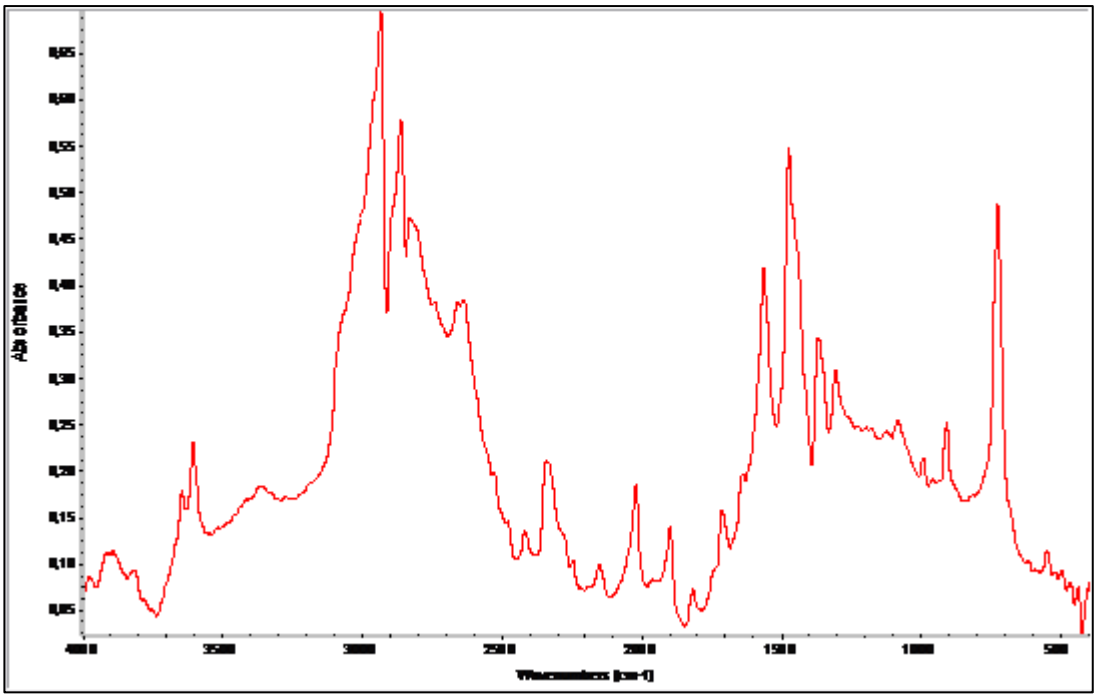


Figure 4.2: Spectrogram of HDPE with 1% Manganese laureate

4.2.3 Experiment 3: Thermal degradation: Pyrolysis of HDPE with 1% Manganese laureate

Objective:

To identify the carbonyl and functional group presence in HDPE

Material:

Solution of HDPE with Manganese laureate

Equipment:

Fixed-bed Pyrex

Methodology:

The fixed-bed Pyrex glass column reactor of apparatus as in Figure 4.3, where the pyrolysis of HDPE was carried out. Liquid pyrolysis yields were collected in a container to analyse by using FTIR Spectroscopy. Spectrogram is generated by Omnic software.

Result:

Spectrogram of thermal degradation of HDPE is show as Figure 4.4.

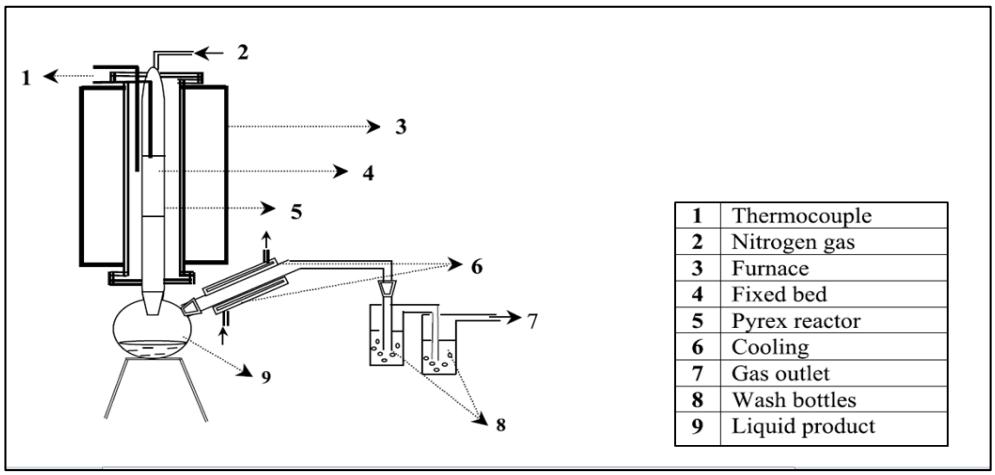


Figure 4.3: Lab-scale fixed-bed pyrolysis experiment set-up [12]

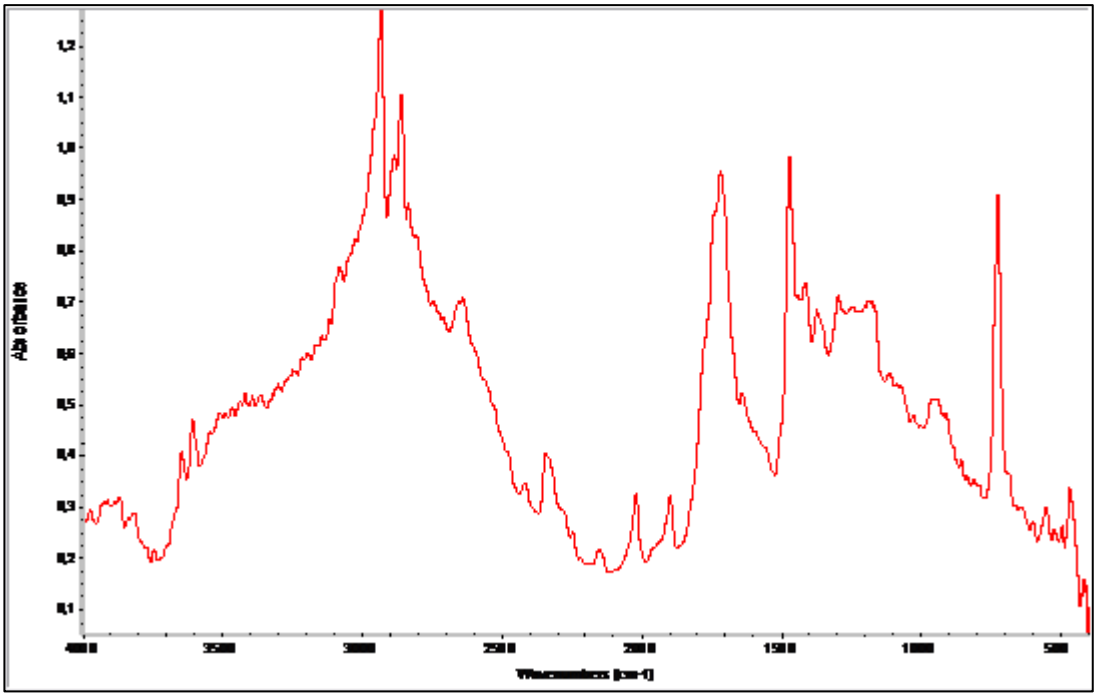
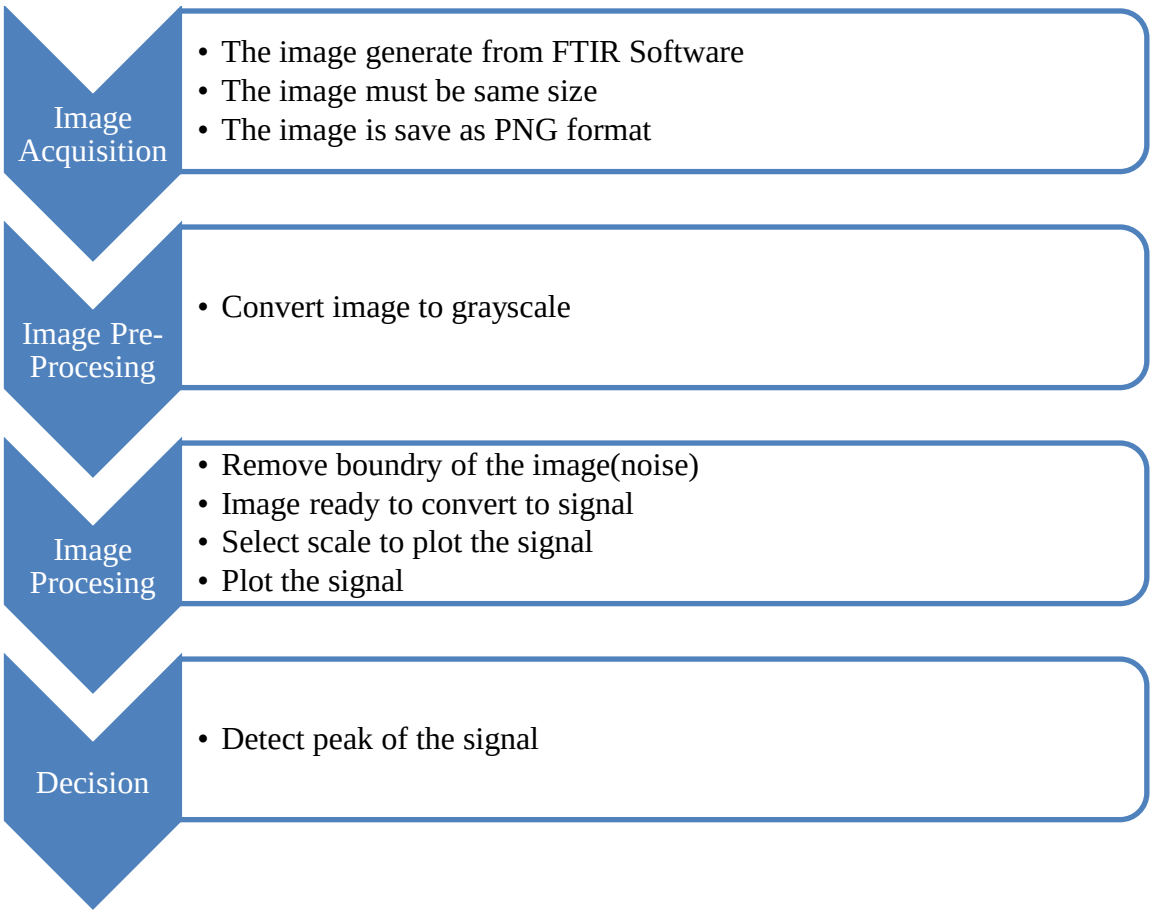


Figure 4.4: Spectrogram of thermal degradation of HDPE

4.3 Software Development

To identify the presence of compound in spectrogram, chemist concern about the presence of peaks in spectrogram. The presence of peaks in spectrogram shows the presence of functional group or compound in a chemical sample [13]. Value of peaks is determined by wavelength (x-axis).

As the spectrogram is in the image format, there is no other way to know the value of peak in spectrogram except converting the spectrogram into signal. In this part, the development of programming coding to convert image into signal by using MATLAB is explained in detail based on Flow Chart 4.1.



Flow Chart 4.1: Software Development process

4.3.1 Image Acquisition

The algorithm is start with image of spectrogram FTIR spectrogram. The format of captured image should be in PNG. In this project, the image must be in same size as easy to make an analysis and comparison with the processing image and original image. The image of spectrogram is as show in Figure 4.5.

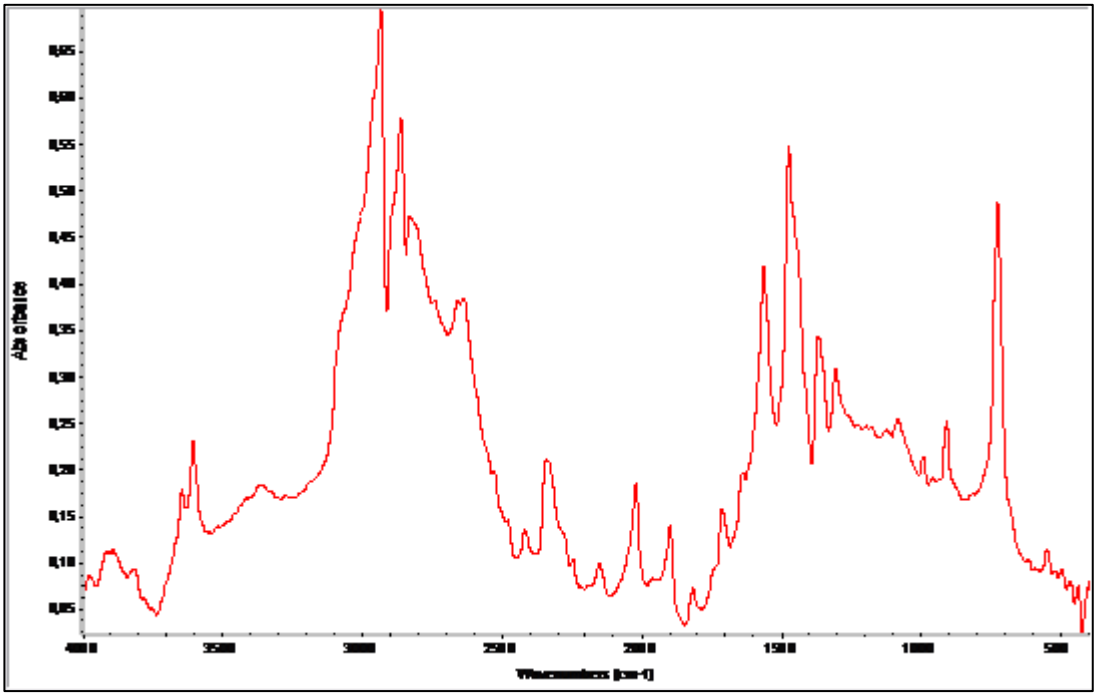


Figure4.5: Image of polyethylene spectrogram

4.3.2 Image Pre-Processing

Next step, the image will be pre-processes to change image into a format readable by MATLAB Software. The image will read from a specific folder by using *imread* function [14]. The original image is a combination of three component of colour arrays where it arrays a represent by red, green and blue. The image which in RGB will convert to 255 gray-scales using rgb2gray function. This process was done to get the pixel value of each component of the colour arrays. The coding is shown in as below. Figure 4.6 is show as original image and Figure 4.7 is show as Gray-scale Image.

```
clear,clc
a=imread('6.png');
figure(1),imshow(a),title('Original Image')
a1=rgb2gray(a);
figure(2),imshow(a1),title('Graycsale Image')
```

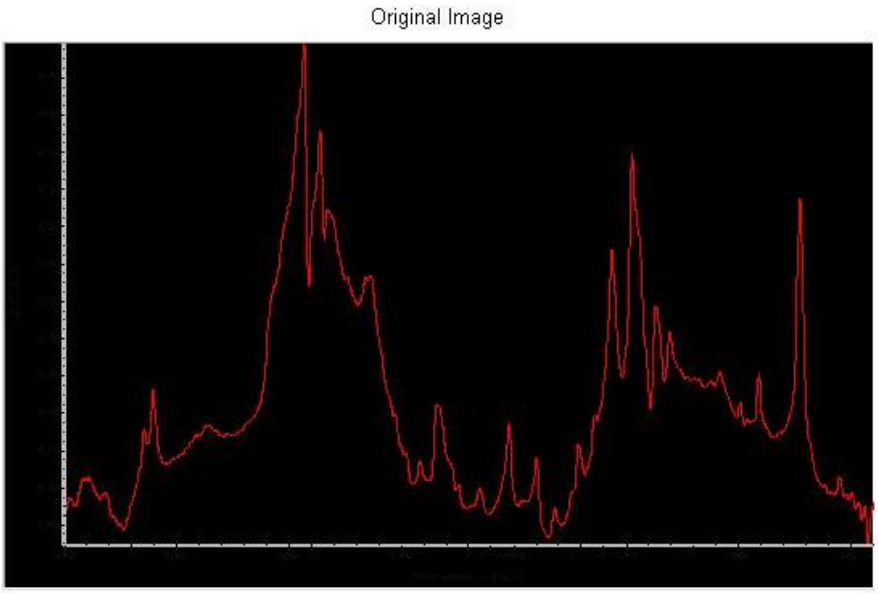


Figure 4.6: Original Image

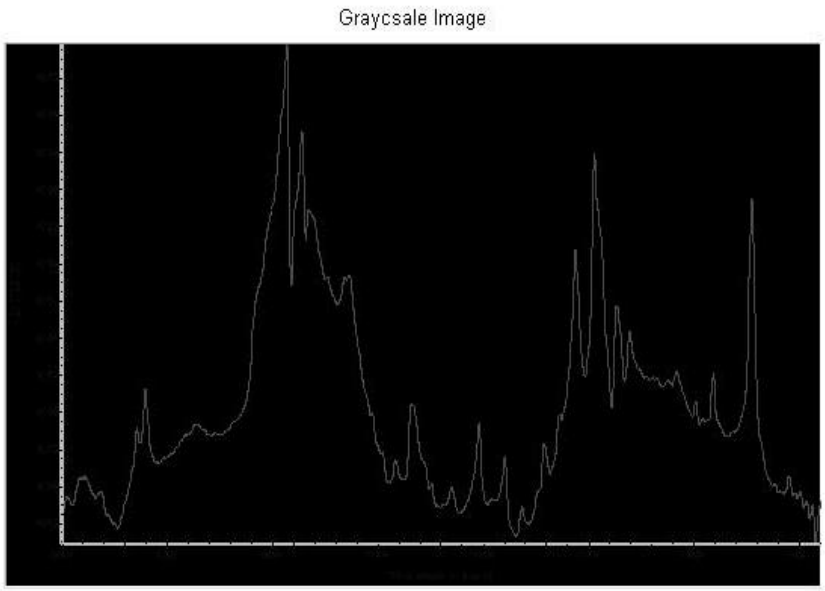


Figure 4.7: Gray-scale Image

4.3.3 Image Processing

There are several steps in image processing part:

4.3.3.1 Remove Noise
4.3.3.2 Find the location of line scale
4.3.3.3 Scale decision
4.3.3.4 Signal Extraction
4.3.3.5 Create the signal

4.3.3.1 Remove Noise

First and foremost, noise in the image should be removed. Image noise is classified as unwanted information of an image [15]. Boundary line in the image as show in Figure 4.8 is identified as noise in the image. In the MATLAB, location of boundary can be display as Matrix as in figure 4.9

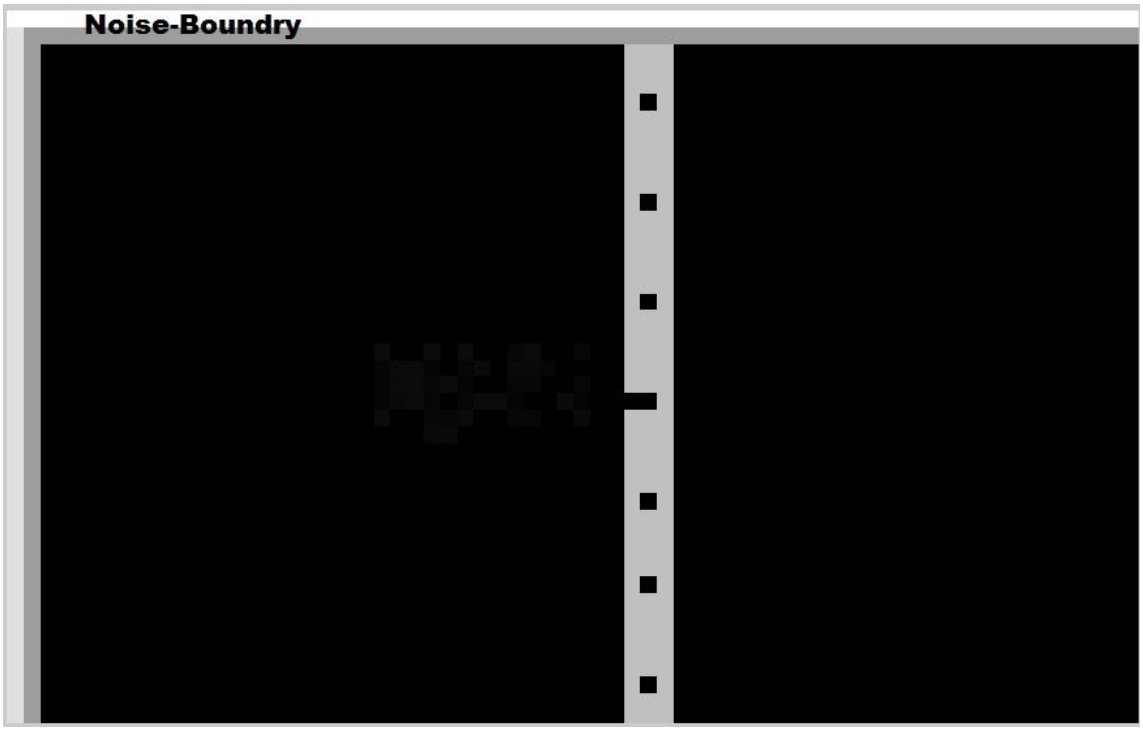


Figure 4.8: Boundary in the image is classify as noise

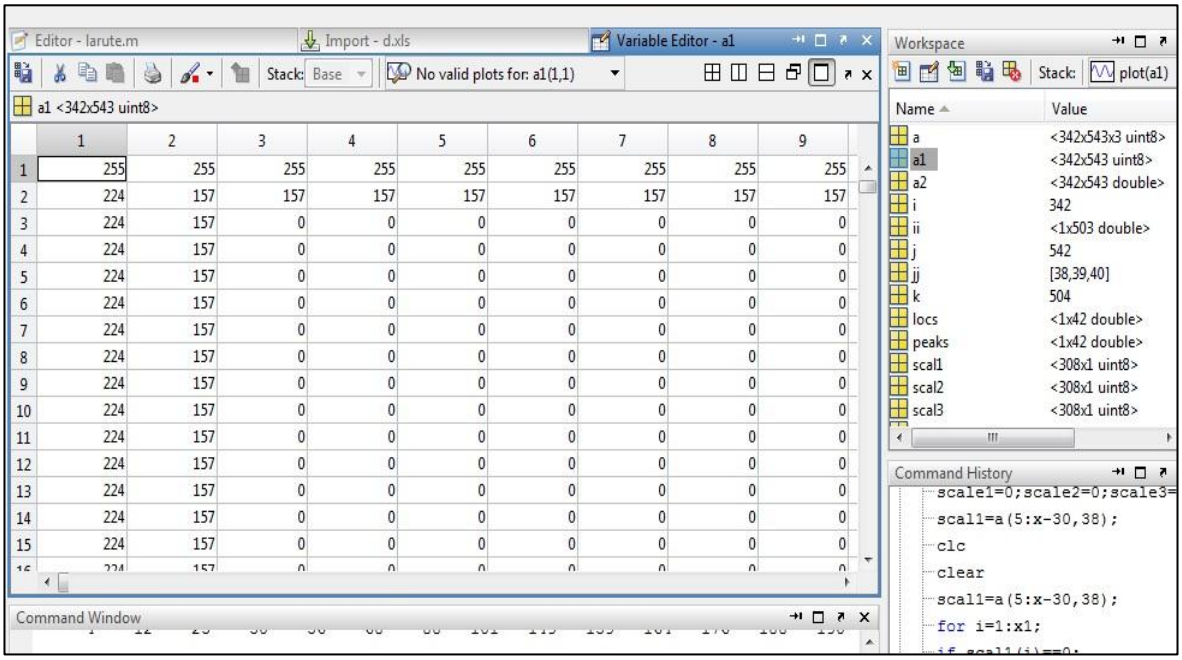


Figure 4.9: Location of boundary in matrix

4.3.3.2 Find location of line scale.

Next is to find the location of line scale in the image. The location is between the boundary and line scale as in Figure 4.10. It can be display as matrix show in Figure 4.11. This part is performed to locate 0 values in the location from boundary line to line scale.

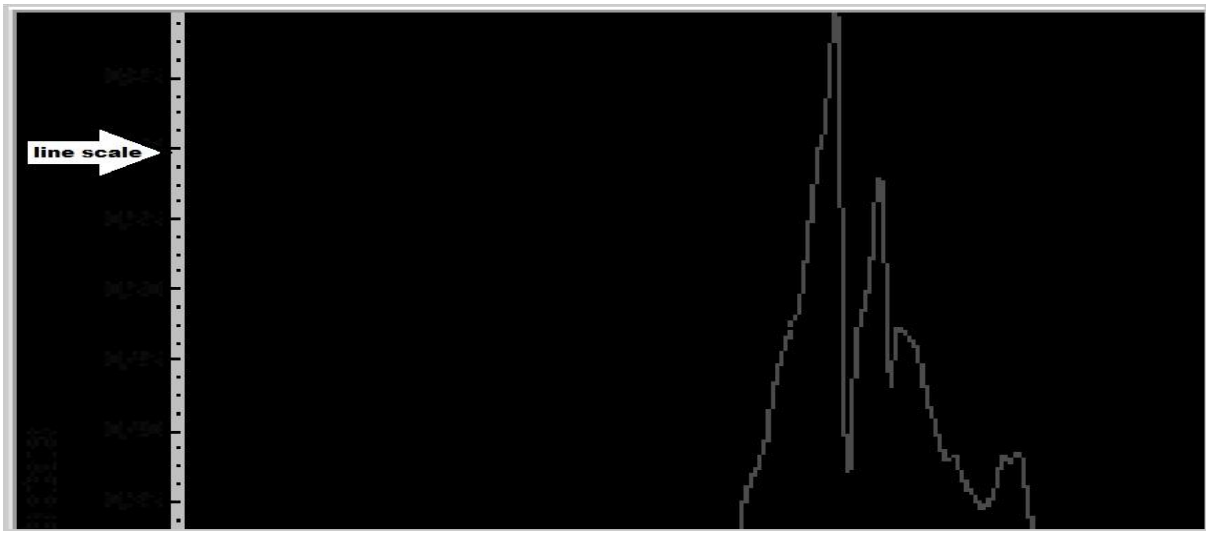


Figure 4.10: Location of line scale in the image

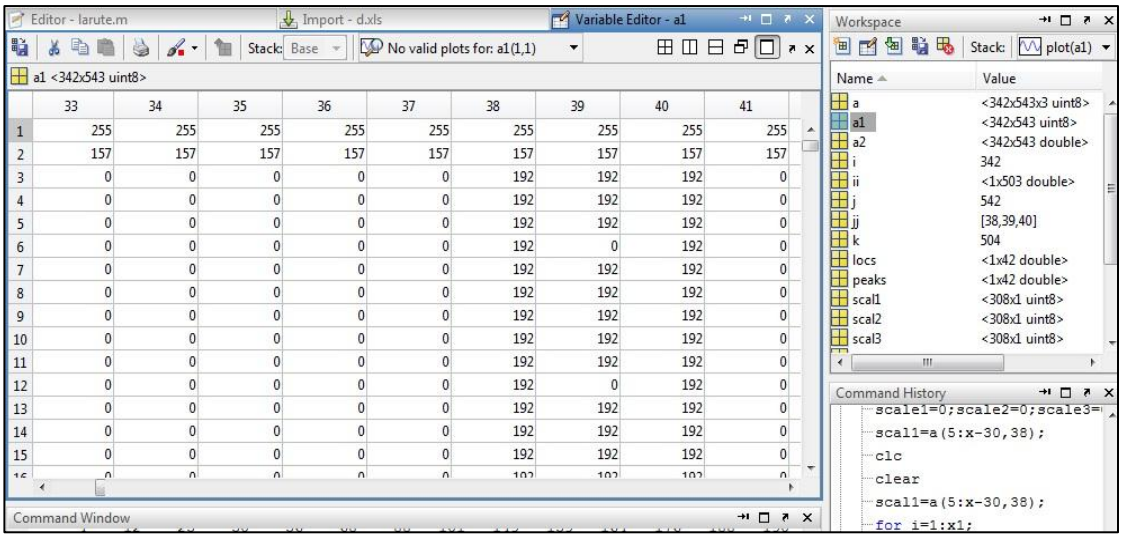


Figure 4.11: Line scale present in matrix

4.3.3.3 Scale decision

To draw the signal, we need scale for x-axis and y-axis. Based on all data/image, each image has same scale for x-axis but different type of scale for y-axis as recorded in Table 4.1. To select scale for y-axis, there are some considerations that need to be review.

Data	y-range	Column 38	Column 39	Column 40
1	0.75	15	61	5
2	0.75	15	61	5
3	1.6	10	83	5
4	0.75	15	61	3
5	1.2	12	49	0
6	0.65	13	53	2
7	1.4	13	51	0
8	1.2	14	71	6

Table 4.1: Scale on y-axis of all data/image

As go through to location of y-axis or line scale, it located at column 38, 39 and 40 as show in Figure 4.11. In the original image of Figure 4.10, the black dot in the line scale have value of zero,0 and others have value of 192 as shown in matrix in Figure 4.11. The different location of black dot in line scale of these 3 columns will lead to select the scale of y-axis. The Figure 4.12, show the zero location in the line scale.

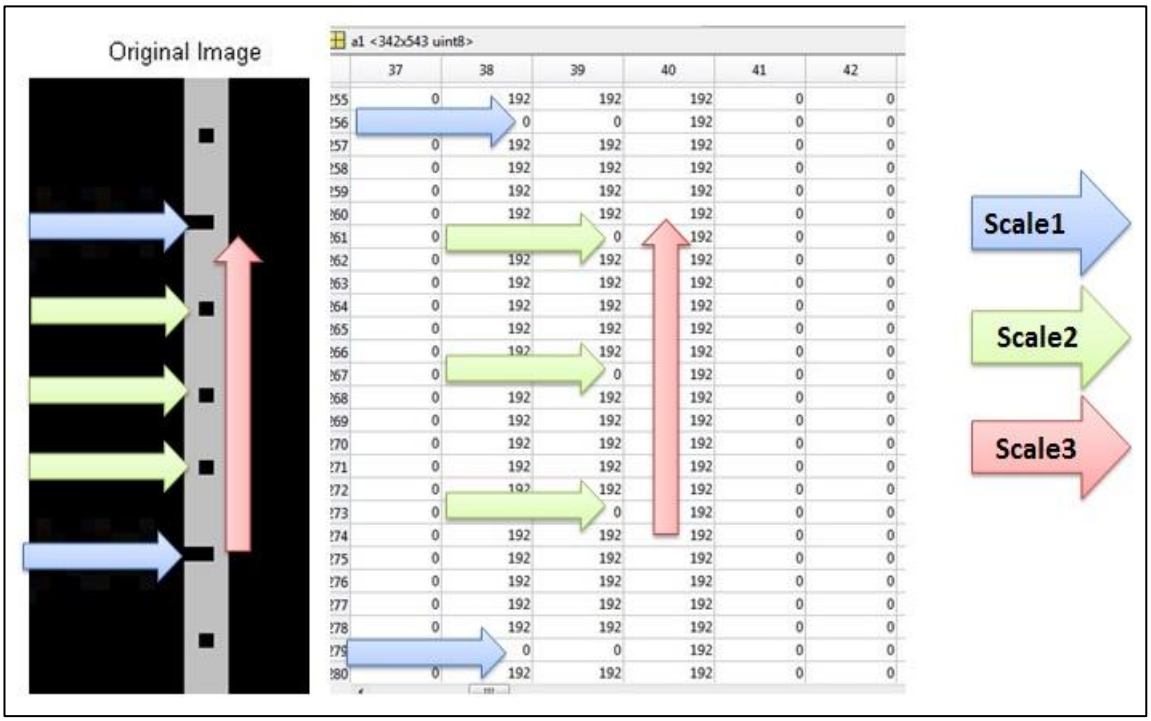


Figure 4.12: Location of zero,0 in column 38,39 and 40

To find total value of zero,0 in the scale line of each column, the coding below is develop.

```
%find the scale line
scal1=a(5:x-30,38);%scan kat setiap baris kat kolum 38
scal2=a(5:x-30,39);% scan kat setiap baris kat kolum 39
scal3=a(5:x-30,40); scan kat setiap baris kat kolum 40
x1=length(scal1);
```

Part 2

```
scale1=0;scale2=0;scale3=0;
for i=1:x1;
if scal1(i)==0;
scale1=scale1+1;
```

Part 3

```
end
if scal2(i)==0;
scale2=scale2+1;
end
if scal3(i)==0;
scale3=scale3+1;
end
end
scale1,scale2,scale3
```

Purpose of Part 2 coding is to read all value of location for each column. Column 38 is assign as *scal1*, column 39 is assign as *scal2* and column 40 name as *scal3*.

```
scal1=a(5:x-30,38);%scan each row at column 38
scal2=a(5:x-30,39);% scan each row at column 39
scal3=a(5:x-30,40); scan each row at column 40
x1=length(scal1);
```

For the 3rd part of coding, when MATLAB found the value of zero,0 in the location of column it will count and recorded. This part is develop to show how many value of zero,0 in each column. This coding is test for all data and recorded as in Table 4.1

The result in the table show that the total value of zeros,0 in column 38 also has related number with value of y-axis. Column 39 it seems has too many numbers of zero and the value is not stable. For Column 40, it has one data there is no zero,0 presence line scale. Based on this assumption, column 38 is choosing as scale for y-axis for the new signal.

4.3.3.4 Signal Extraction

First, the background is paint with white colour by using *ones* function [16]. This function will cause the entire image in white pixel. Based on matrix of image,

value of red pixel is between 30 until 100. Any value in this range will set to 0 as the black dots. In a column, there must be different value in a set of sequence of number as in Figure 4.13. In this case, only a value will choose to be plot. In the coding, *round* function is used to find mean point for each column. Coding in Part 4 will function as discuss in this part. The result after run the coding of Part 4 as show in Figure 4.14

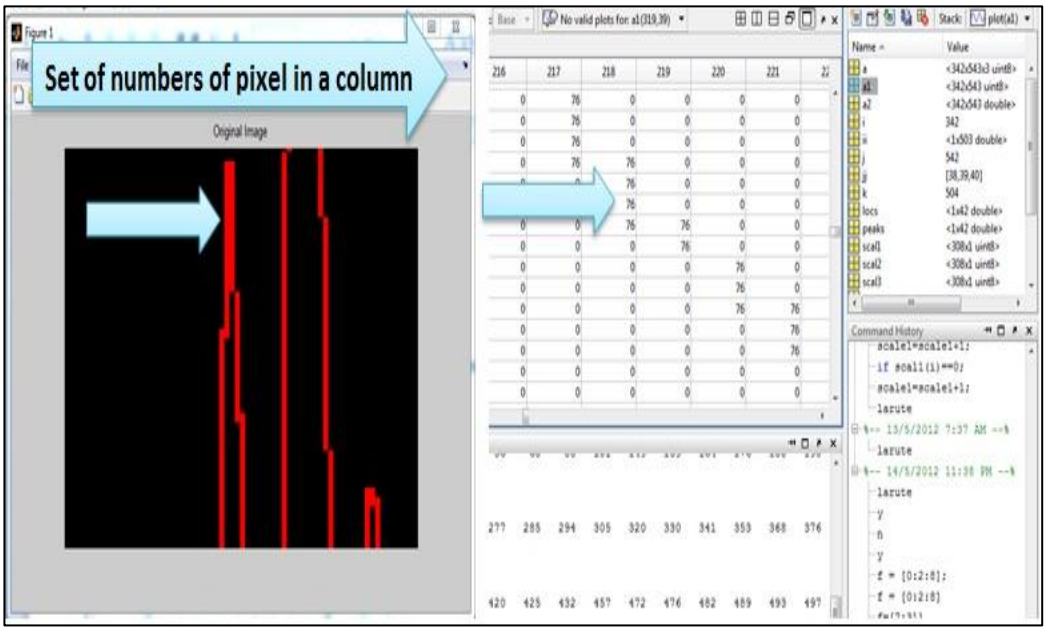


Figure 4.13: Set of sequence number in a column

```
%for signal
a2=a1;a2=ones(x,y);%paint the image to white colour
for j=1:y;
k=0;ii=1;
for i=1:x;
if (a1(i,j)>=30)&(a1(i,j)<=100);
k=k+1;
ii=i;
end
end
ii=round(ii-(k/2));%find mean point for each column
a2(ii,j)=0;%locate the black dote on the mean point location
end
Figure(3), imshow(a2),title('extract the signal')
```

Part 4

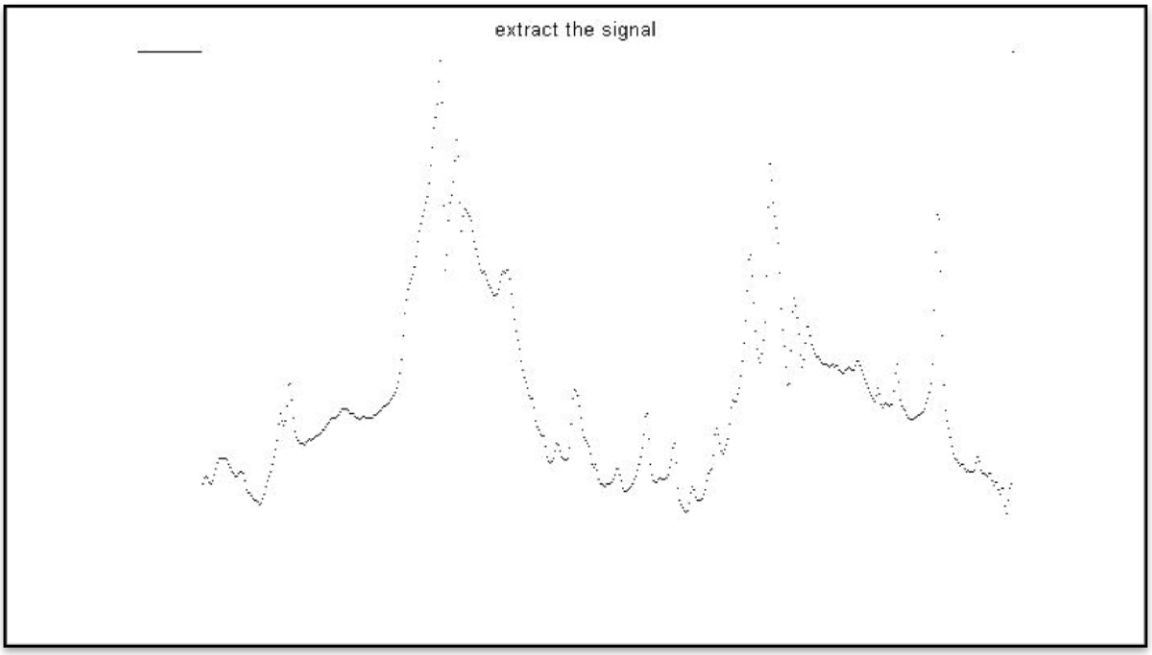


Figure 4.14: Image after perform coding part 4

4.3.3.5 Create the signal

Create the signal is the last stage of image processing. Process will start with read the value start from column 40 until 542 in every row. If the MATLAB found location contain value of zero,0, the location will be recorded. Then the location is plotted as signal as result in Figure 4.15 after coding Part 5 is run in MATLAB.

```
[x,y]=size(a2);
k=1;
for j=40:y-1;%start from column 40
for i=1:x;
if a2(i,j)==0;%record the location of the black dot
ii(k)=x-i;
k=k+1;
end
end
end
figure(4),plot(ii)
```

Part 5

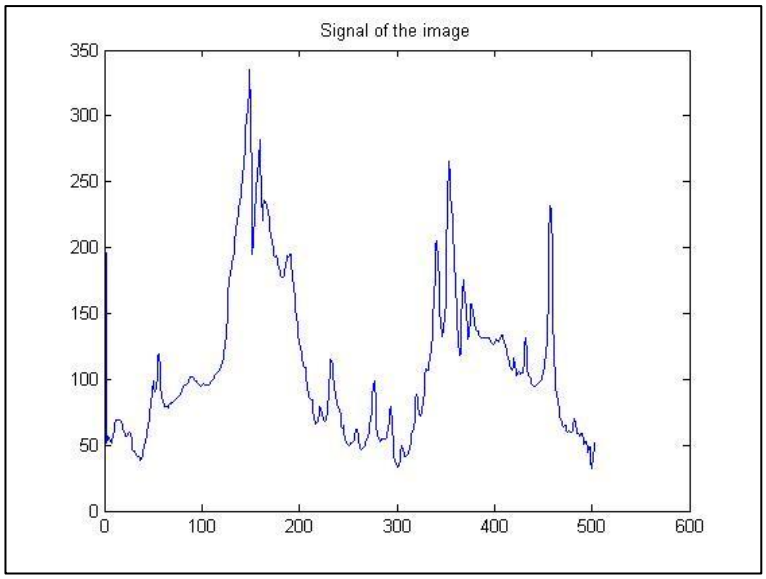


Figure 4.15: Signal image of spectrum

4.4 Decision

The main of extract the image to signal is to detect the peak of the signal. The peak of signal is show the fundamental of polyethylene. Peak of the signal can be determined by using [*peaks locs]* function in MATLAB [17]. The result to find peak is shown as in Figure 4.16. Peak and it location is recorded in Table 4.2

```
[peaks locs] = findpeaks(ii)
hold on;
plot(locs,peaks,'o','MarkerEdgeColor','r')

locs=locs';
range=xlsread('ch.xlsx');
max=size(range);
range(max(1)+1)=0;
result=range(locs+1)
```

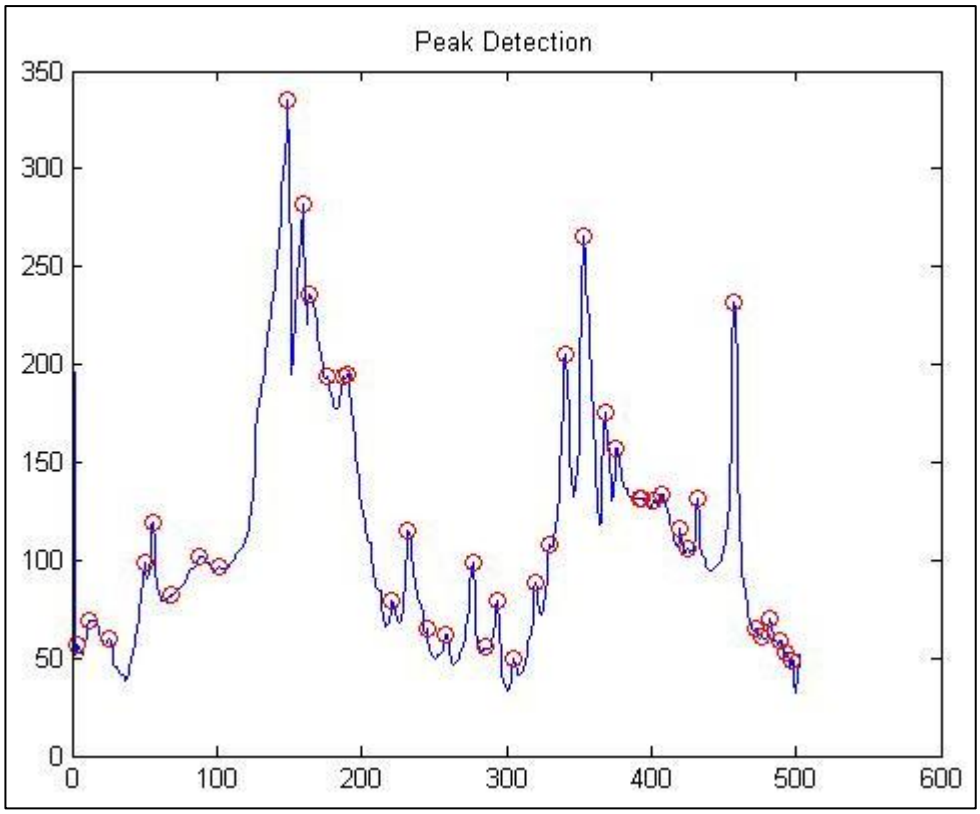


Figure 4.16: Peak Detection

4.5 Development of Library

4.5.1 Corresponding Wavenumber

After create the signal, the identification of functional group or bonding group is based on Wavenumber, cm^{-1} at x-axis. Each chemical fundamental have their corresponding absorbance bands [18]. Aim for converting the image of spectrogram into signal is to read the value of peak in x-axis as Wavenumber, cm^{-1}.

Refer to image of spectrogram in Figure 4.17, the wavenumber, cm^{-1} (x-axis) is starting at 4000-500cm^{-1}

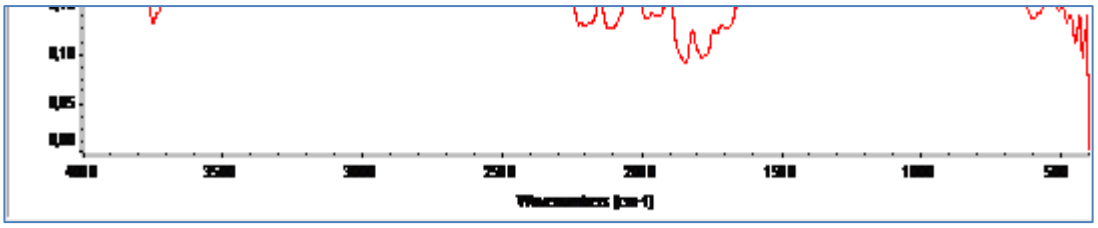


Figure 4.17: Scale of x-axis Spectrogram is from 4000-500 cm^{-1}

The signal that has been plotted is in range 0-500 cm^{-1} at x-axis as shown in Figure 4.18.

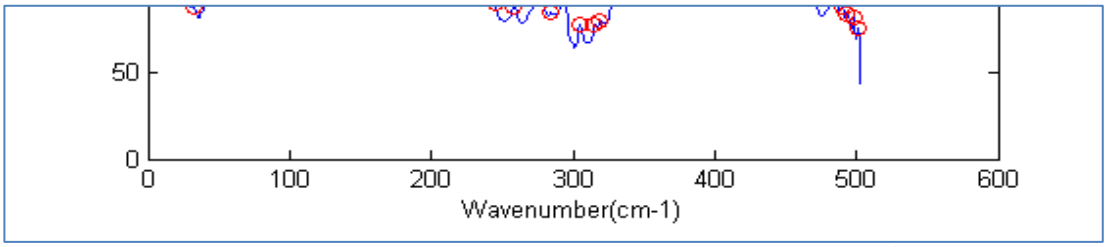


Figure 4.18: Scale of x-axis Signal is from 0-500 cm^{-1}

Later, when get the value of peaks in x-axis, the value is in range of 0-500cm^{-1}. As mentioned, FTIR is operating in infrared range which 4000-500cm^{-1} [19]. In solution, value of x-axis the signal must be compared to value of x-axis of spectrogram.

Table 4.2: Ratio between scale Signal and Spectrogram at x-axis

Signal x-axis, cm^{-1}	Spectrogram x-axis, cm^{-1}
0	4000
100	3500
200	3000
300	2500
400	2000
600	1500
	1000
	500
6	**8**

Table 4.2 show the ratio between two scales is 3:4. It shows that, the number of numbers present is not linear. Moreover, this type of information does not really help to find the solution.

Table 4.3: Ratio the number of numbers presence in range

0-500	Range x-axis	4000-500
500	The number of numbers in range presence	3500
1	Ratio	7

Another method is determined the number of numbers in the range of both scale. The data in Table 4.3 show that, a number in x-axis signal represent as 7 numbers in x-axis of spectrogram. Based on this idea the library for this system can be build. In this library, x-axis of signal is assign as wavenumber,cm-1 and x-axis of spectrogram is assign as Corresponding Waveform,cm^{-1}.

X-axis Signal = Wavenumber

X-axis Spectrogram = Corresponding Waveform

The library of comparison between this x-axis is Show as *Appendix A.* The example for the representation of x-axis if signal and x-axis Spectrogram is shown in Table 4.4. This library will save as excel format and will be used in MATLAB.

Table 4.4: Library of X-axis signal and its Corresponding Range

X-axis of signal	X-axis of Spectrogram	Range
0	4000	4000
1	3993	3999-3993
2	3986	3392-3986
3	3979	3985-3979
4	3972	3978-3972
5	3965	3973-3966

4.3.2 Functional group

Each of chemical components has their own corresponding band. To detect atomically presence of functional group and CH bonding in this project, a library should be developed. The development of Functional group and CH is based on Table 4.5 and Table 1 in Figure 4.6. The library is save in excel format and use in Matlab programming. This library is called as 'fingerprint'. The data of library is show as *Appendix A.*

Table 4.5: 'Fingerprint' Presence of Functional Group based on Band Range (Wavenumber, cm^{-1}) [19]

Wavenumber ,cm-1	Corresponding Band	Functional Group
3300-2500 cm^{-1}	ACID	O-H
1100-1300 cm^{-1}		C-O
1300-1000 cm^{-1}	ESTER	C-O
2850 cm^{-1} and 2750 cm^{-1}	ALDEHYDE	C-H
900-1000 cm-1	-	VINYL
1600-1800cm-1	CARBONYL	C=O

TABLE I. Infrared spectrum and assignments for polyethylene.

Frequency, cm^{-1}	Intensity	Polarization	Assignment[a]
2959	w(sh)	···	$\nu_a(CH_3)$
2925	vs	σ	$\nu_a(CH_2)$[c]
2874[b]	vw	···	$\nu_s(CH_3)$
2853	s	σ	$\nu_s(CH_2)$[d]
2640	w	σ	
2295	vw	σ	
2130	vvw	σ	
2010	vw	π	1303+721=2024
1890	vw	σ	
1805	vvw	π	
1710	vw	σ	
1470[b]	s	σ	$\delta(CH_2)$
1460	s	σ	
1456[b]	vw	···	$\delta_a(CH_3)$
1375	m	π(?)	$\delta_s(CH_3)$
1369	w	π	$\gamma_w(CH_2)$
1353	w	π	$\gamma_w(CH_2)$ amorphous regions
1303	w	π	$\gamma_w(CH_2)$ amorphous regions
1170	vvw	π	
1150	vvw	π	
1110	vvw	π	
1080	vw	σ	ν(CC) amorphous regions
1065	vw(sh)	σ	ν(CC)
965	vvw	···	
888	vw	σ	$\gamma_r(CH_3)$
731	m	σ	$\gamma_r(CH_2)$
721	s	σ	
600	vw	···	
543	w	···	
200	vw	···	

Figure 4.6: Table 1 Infrared spectrum and assignments for Polyethylene [19]

CHAPTER 5

RESULT AND DISCUSSION

5.1 GUI System

The GUI system is develop as interface between the user and internal program (Matlab coding). The GUI will help user load image of spectrogram and the result will present directly in GUI panel. In this part, how user can use GUI system will be discuss.

5.1.1) GUI Panel

In this panel, there is 5 bottons. Button Red, Green and Pink is for load the image. In methodology has been discussed, there are three types of experiment and also have different objective. Figure 5.11 is the panel of GUI.

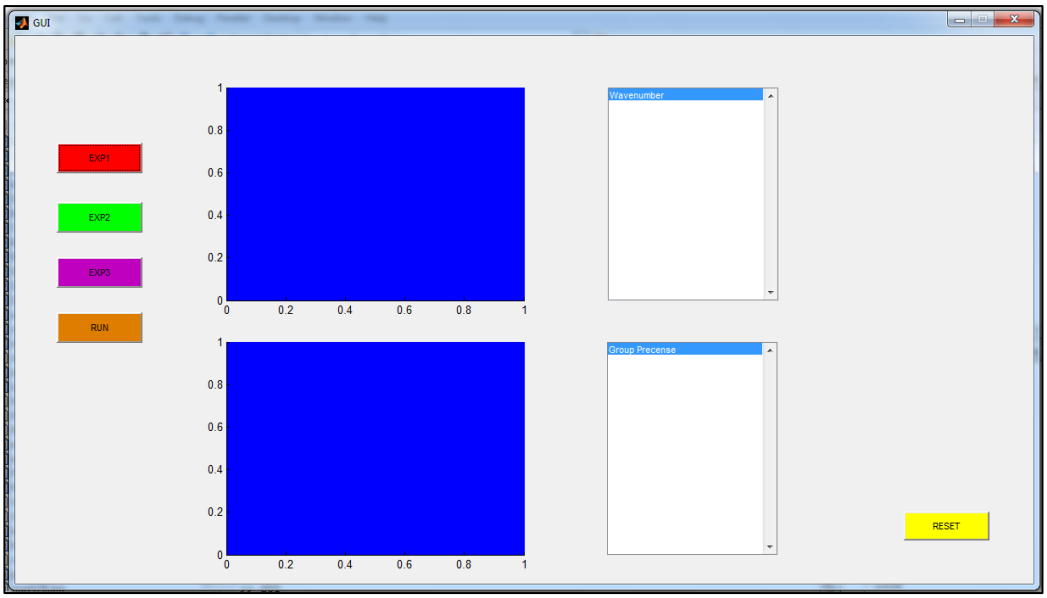


Figure 5.11: GUI Panel

5.1.2) When click button RED (EXP1), the user need to select imae of sectrogram as shown in Figure 5.12. After choose the image, the image will be display at 1st blue box. As in Figure 5.13.

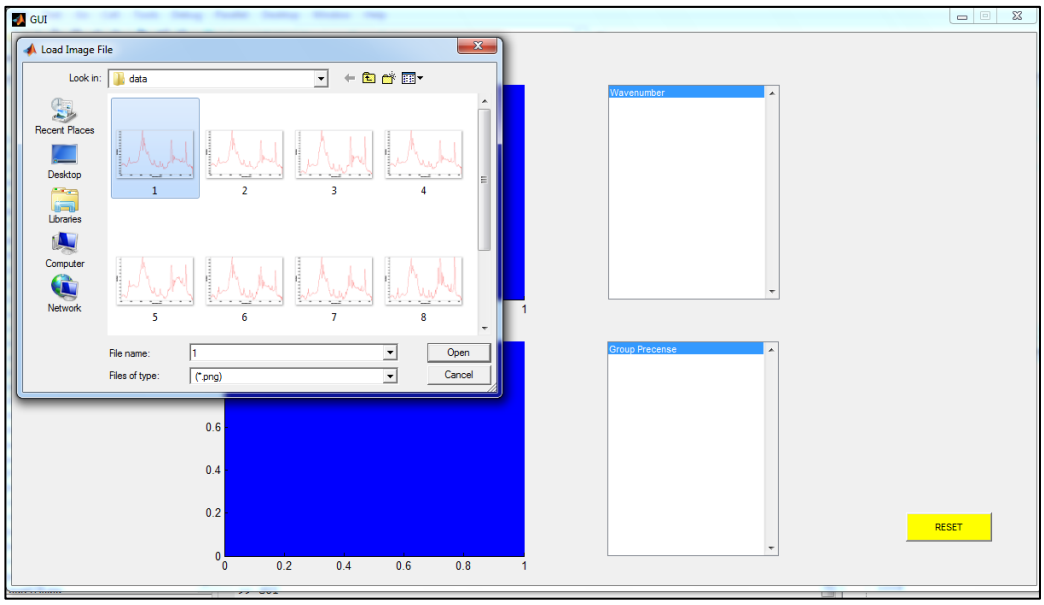


Figure 5.12: User need to choose the data

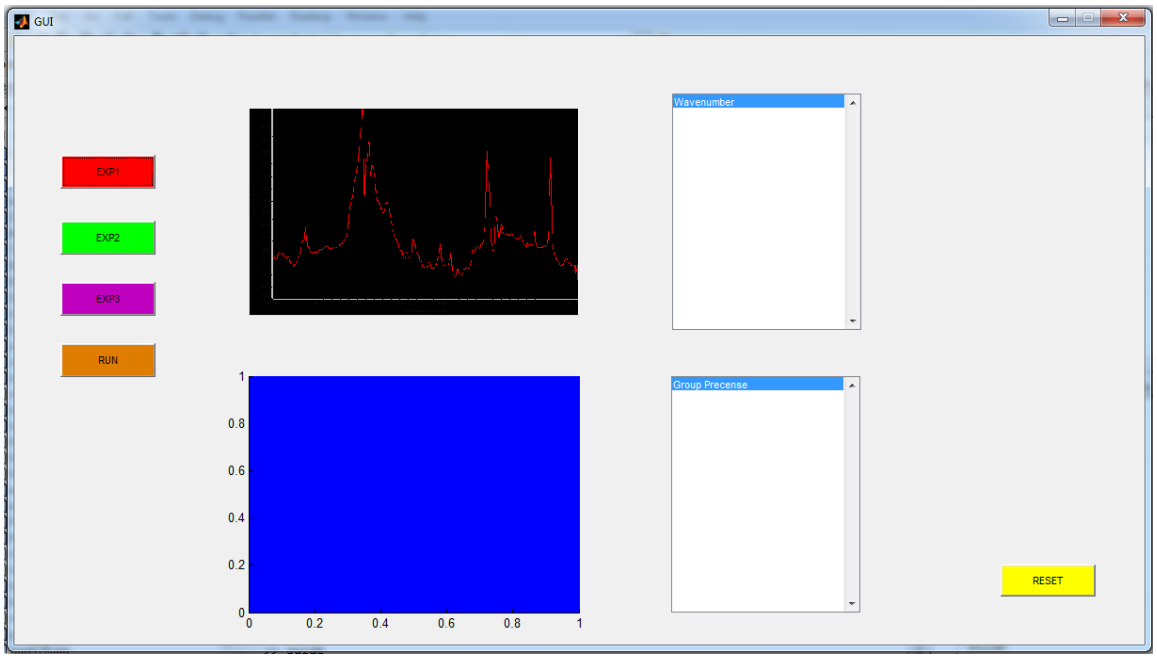


Figure 5.13: The original image will display at 1st box

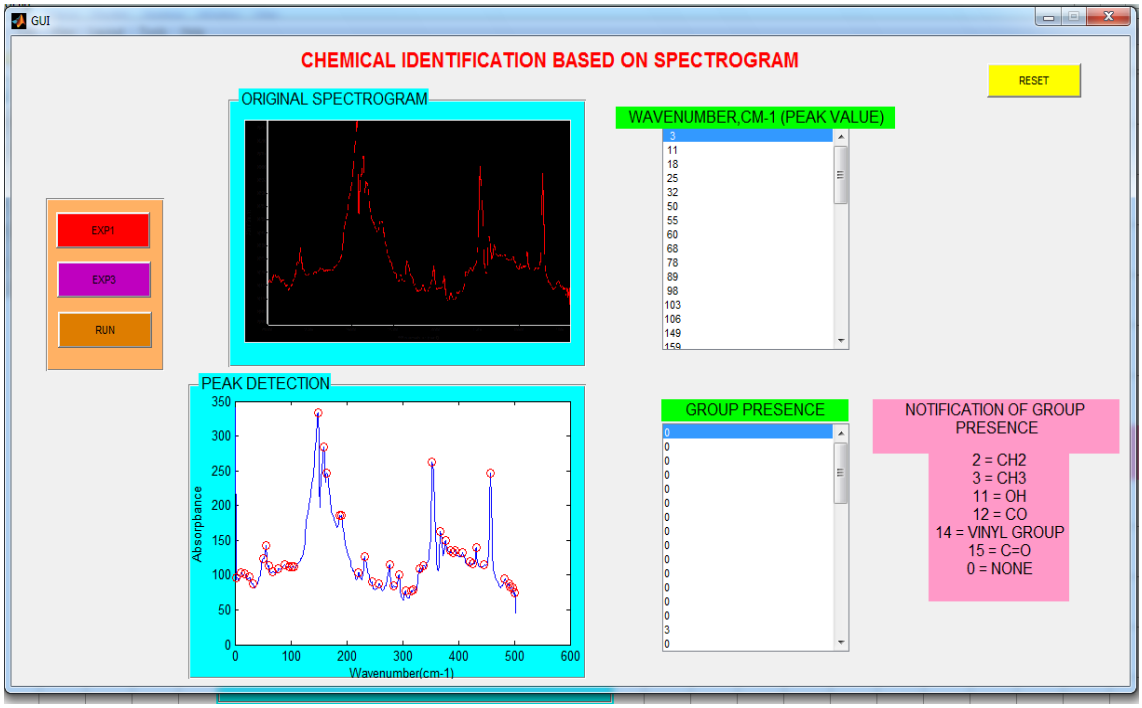


Figure 5.14: The signal, List of Wavenumber, cm^{-1} and List of Functional group will be display in the GUI panel

5.1.3) After that, click the RUN button. The panel will display as Figure 5.14. User can record the List of Wavenumber and Functional Group.

5.1.4) To use with another data, click RESET (yellow) button and the system will ready to use.

5.2 Experiment 1 - Interpreted of Polyethylene

Figure 5.21, Figure 5.22, and Figure 5.23, show the signal of spectrogram from Data 1, Data 2 and Data 3. The experiment is carried out 3rd times to found the acceptable presence of CH group in Polyethylene. Table 5.21.5.22.5.23, are value of peak (wavenumber) and presence of CH in polyethylene.

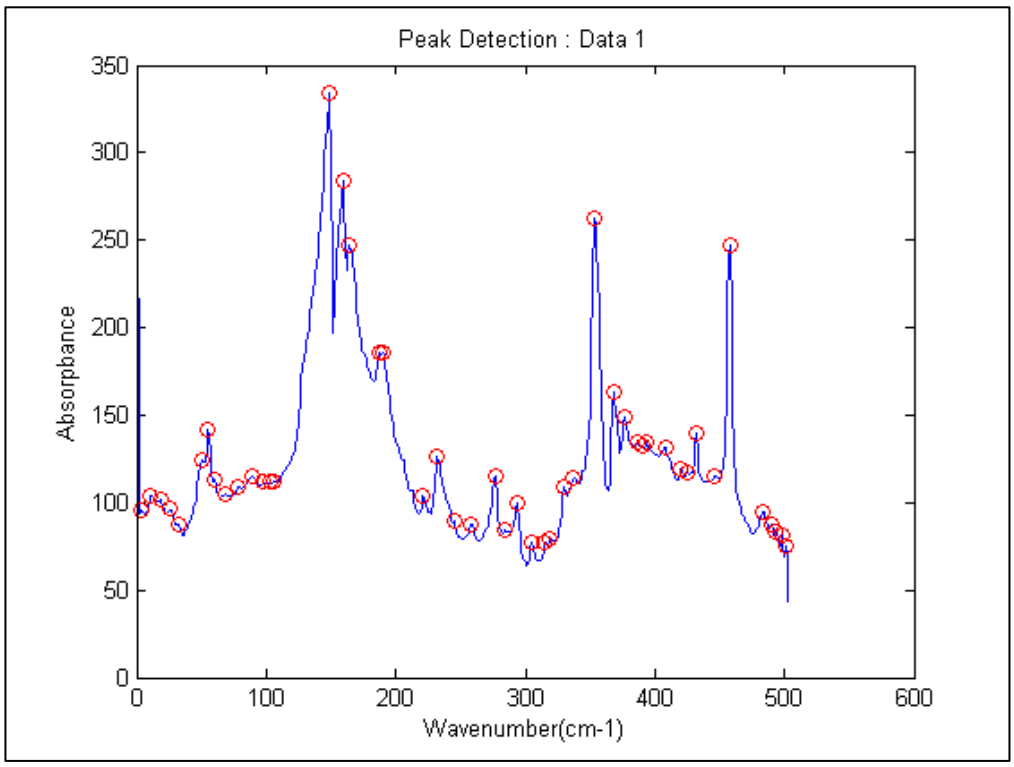


Figure 5.21: Peak Detection of Signal 1

Table 5.21: Presence of CH group Signal 1

Wavenumber cm^{-1}	Presence of CH group	Wavenumber cm^{-1}	Presence of CH group
3	0	277	0
11	0	284	0
18	0	294	0
25	0	305	0
32	0	315	0
50	0	319	0
55	0	330	0
60	0	337	0
68	0	353	0
78	0	368	0
89	0	377	0
98	0	386	CH_2
103	0	390	0
106	0	394	0
149	CH_3	408	0
159	0	420	0
164	CH_2	425	0
188	0	432	0
190	0	446	0
221	0	458	0
232	0	483	0
245	0	490	0
258	0	493	0

According to Table 5.21, there are two groups of CH_2 and a group of CH_3 presence in the first time experiment was carried out. CH_2 is presence at 164cm^{-1} and 386cm^{-1} respectively. Else, CH_3 group is presence at 149cm^{-1}.

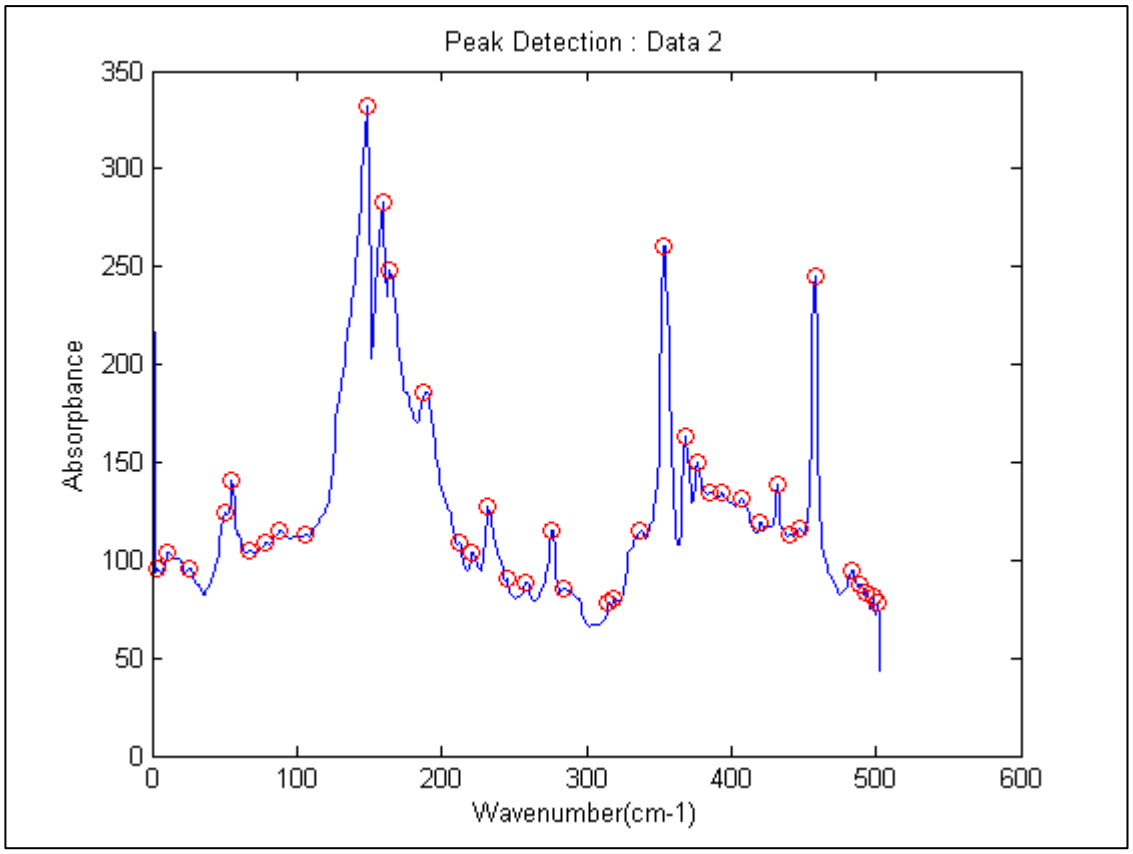


Figure 5.22: Peak Detection of Signal 2

Second time carried out the experiment show that only a group CH_2 is presence. Compare to result in Table 5.21, there are three groups of CH has been detected. Moreover, the presence of CH_2 in Signal 2 is detected at $164cm^{-1}$ as show in Table 5.22 is same as result in Signal 1.

Table 5.22: Presence of CH group Signal 2

DATA 2			
Wavenumber, cm^{-1}	Presence of CH group	Wavenumber, cm^{-1}	Presence of CH group
3	0	284	0
11	0	315	0
25	0	319	0
50	0	337	0
55	0	353	0
67	0	368	0
78	0	377	0
88	0	385	0
106	0	394	0
148	0	407	0
159	0	420	0
164	CH_2	432	0
188	0	441	0
212	0	447	0
221	0	458	0
232	0	483	0
245	0	489	0
258	0	493	0
276	0	498	0

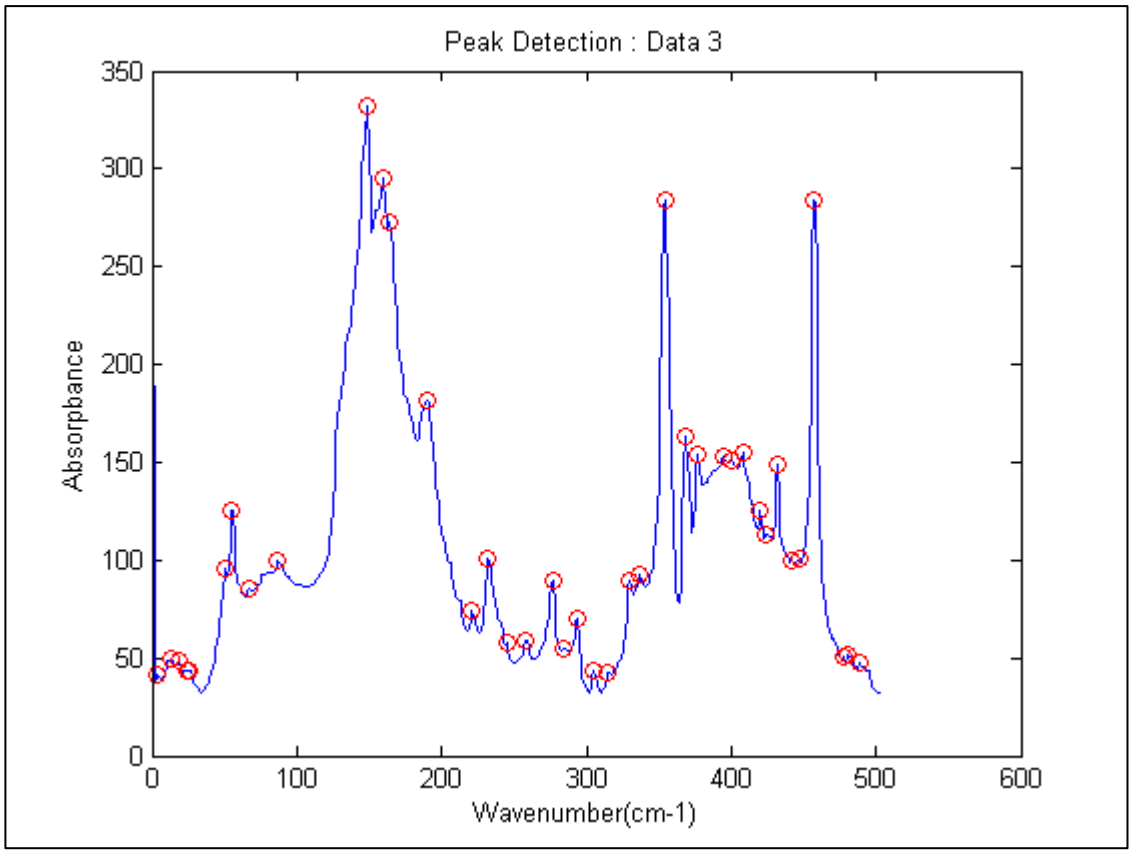


Figure 5.23: Peak Detection of Signal 3

The result in 3rd time of carried out the experiment show that there are two groups of CH_2 have been detected. CH_2 group is presence at 164 cm^{-1} and 386cm^{-1} based on result in Table 5.13. The presence of CH_2 at 164cm^{-1} is prove as same as Signal 1 and Signal 2. The presence of CH_2 at 386cm^{-1} in Signal 3 is same result s Signal 1. Table 5.23 show the result of presence CH_2 group in polyethylene.

Table 5.23: Presence of CH group Signal 3

DATA 3			
Wavenumber cm^{-1}	Presence of CH group	Wavenumber cm^{-1}	Presence of CH group
4	0	305	0
11	0	315	0
25	0	330	0
50	0	337	0
55	0	353	0
68	0	368	0
78	0	377	0
88	0	386	CH_2
98	0	394	0
148	0	408	0
159	0	420	0
164	CH_2	432	0
188	0	441	0
221	0	447	0
232	0	458	0
245	0	483	0
258	0	489	0
276	0	493	0
284	0	498	0
293	0		

Table 5.24: Presence of CH group from Data 1 to Data 3

DATA	Wavenumber, cm^{-1}	Presence of CH group
DATA 1	149	CH_3
	164	CH_2
	386	CH_2
DATA 2	164	CH_2
DATA 3	164	CH_2
	386	CH_2

Table 5.24 is summarizing of all result from Signal 1, Signal 2 and Signal 3. Presence of CH_2 at $164cm^{-1}$ has been prove by all the experiment, and presence CH_2 at 386 is prove by 1^{st} and 3^{rd} time carried out the experiments. Group of CH_3 only presence once out of three times carried out of the experiment. Even though, the presence of CH_3 in polyethylene should be considered as the CH3 group presence not overlap with other group at $149cm^{-1}$.

Before finalize the presence of CH group in this experiment, the presence of CH at should be compare to library in *Appendix A*.

Table 5.25 Comparison wavenumber of Signal and its corresponding range

Wavenumber, cm^{-1}	Correspondent Wavenumber cm^{-1}	CH group	'fingerprint' of CH Wavenumber, cm^{-1}
149	2963-2957	CH_3	2959
164	2858-2852	CH_2	2853
386	1304-1298	CH_2	1303

As refer to range of 'fingerprint' of CH group in infrared spectrum, its present in all Correspondent Wavenumber, cm^{-1} range as Table 5.15. It can be conclude, in the spectrum, the CH_3 is presence between 2963 cm^{-1} – 2957 cm^{-1} and at 149cm-^{1} in the signal. CH_2 is presence in two bands in spectrum at 2858 cm^{-1} – 2852 cm^{-1} and 1304 cm^{-1} – 1298cm^{-1} at 164cm^{-1} and 386cm^{-1} respectively in the signal.

The presence of CH_2 and CH_3 in this wavenumber (cm^{-1}) as show the in the Table 5.15 prove the fundamental of polyethylene.

5.3 Experiment 2 -Interpreted of presence of 1% Manganese Laureate in HDPE

For the second part, 1% Manganese laureate is adding to HDPE. Figure 5.31 is a signal for presence of HDPE only. After the addition Manganese in HDPE, the spectra undergo slight change as in Figure 5.32.

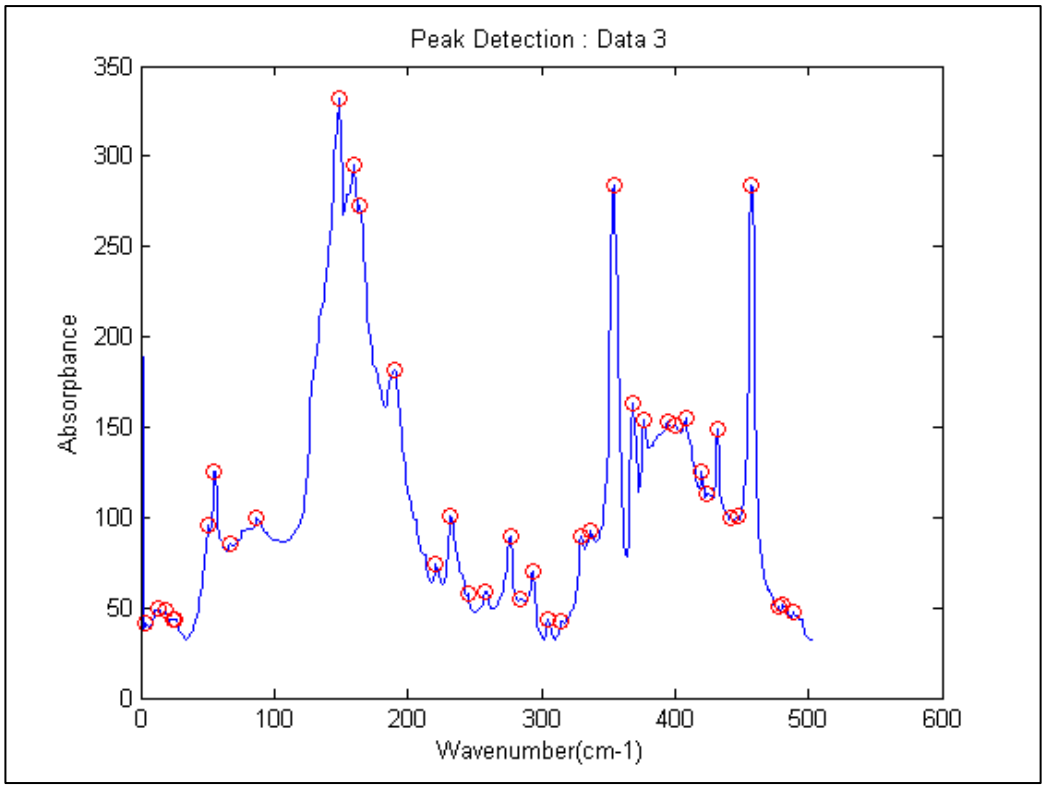


Figure5.31: Signal of HDPE

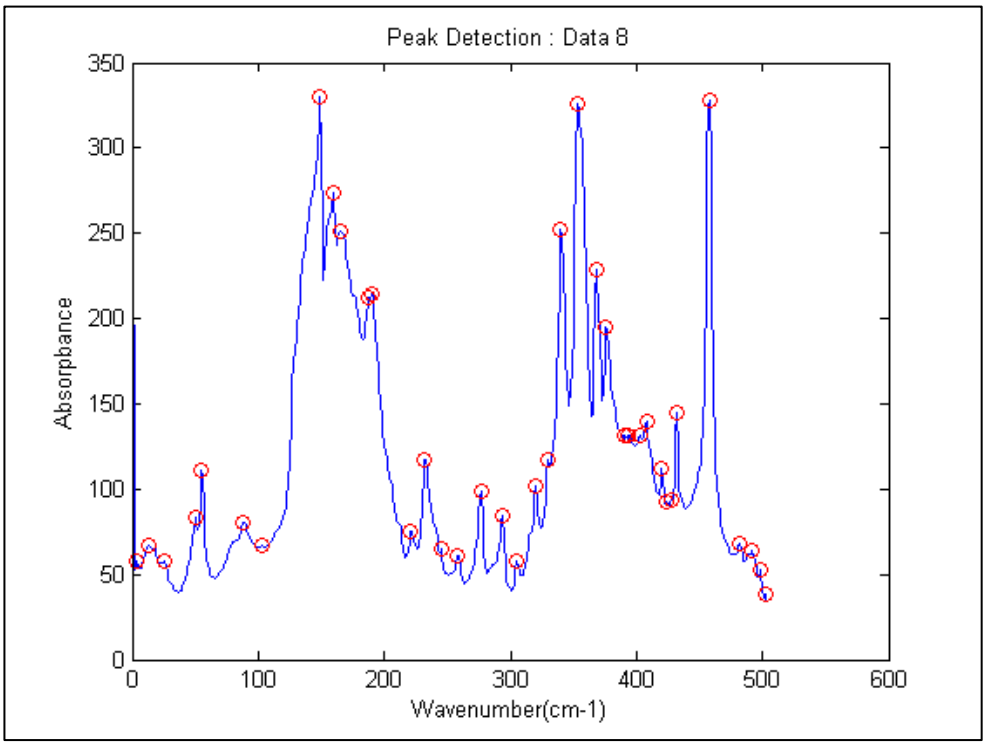


Figure 5.32: Signal of HDPE with 1% Manganese Laureate

In this part, the difference spectra of HDPE after addition of Manganese laureate need to be identify. Furthermore, the appearance of Manganese compound in HDPE needs to be assigned. By plotting the HDPE signal and HDPE with addition of Manganese laureate signal in a graph, it clearly show that signal of HDPE with Manganese laureate have surplus peak compare to signal with HDPE only. The Figure 5.33 show the appearance of surplus peak of signal HDPE with Manganese laureate at 340cm^{-1}. It can conclude that the surplus peak in this signal indicate the present of Manganese.

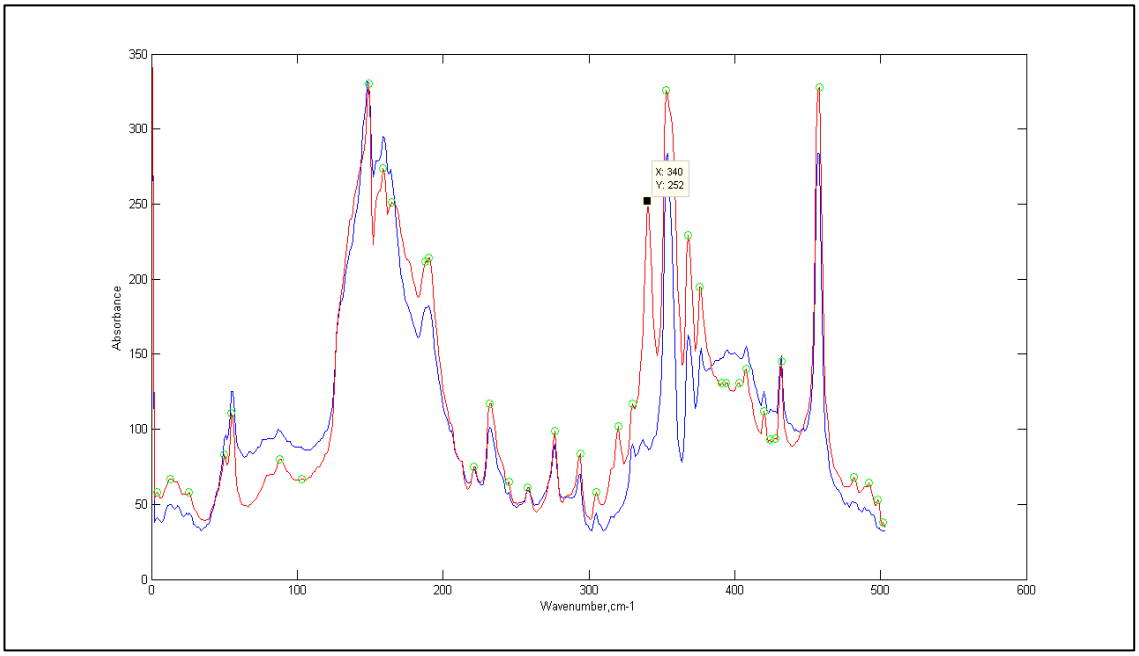


Figure 5.33: Comparison between two signals, blue signal is present of polyethylene and red signal represent signal for polyethylene with 1% Manganese Laureate. A surplus peak appears at 340cm^{-1}.

Another way to determine the presence of Manganese by performs the idea of different spectra [3]. Based on this idea, we can find the different between two signals. It performs by subtracting the two signals, between HDPE and HDPE with Manganese laureate.

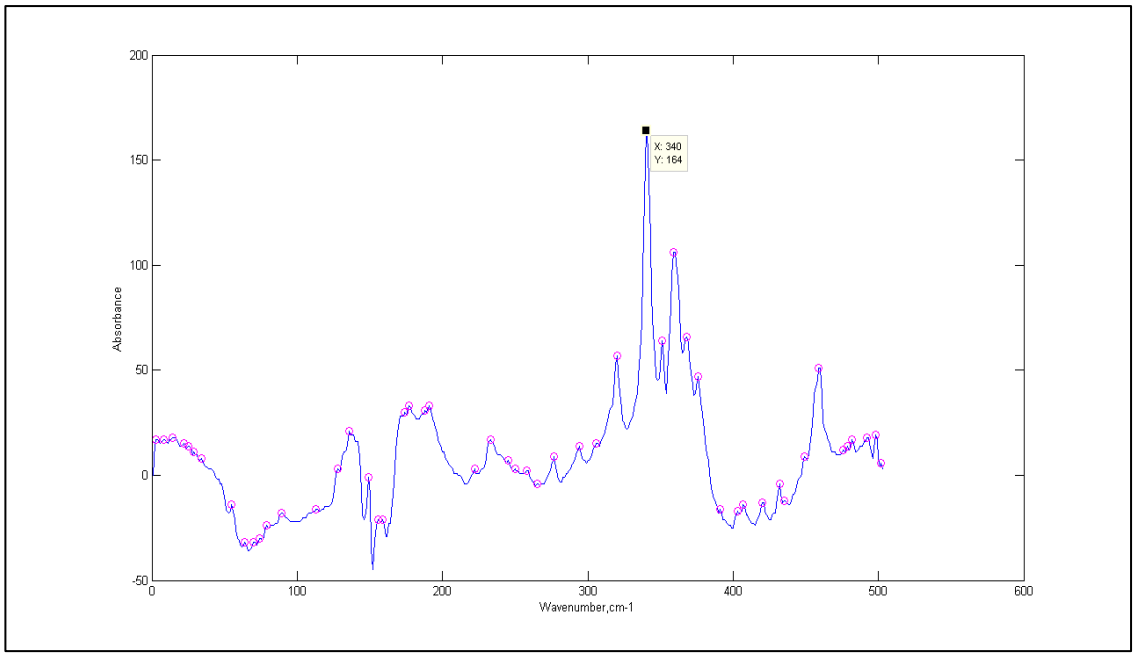


Figure 2.34: Result of different between two signals

After find the difference between two signals, it shows that some changes values of each peak as show in Figure 2.34. As state before, the signal of HDPE with Manganese will have surplus of peaks compare to signal with HDPE only. As result in Figure 2.34, peak at 340cm^{-1} seem to be the one that experience a slight decline compare to others peaks. By comparing this peak to its original signal in Figure 5.31, it proved the presence of Manganese.

Manganese does not have specific range or absorption band in infrared spectrum. Addition of Manganese in HDPE is to act as catalyst. This experiment is carried out to determine the presence of Manganese. Therefore, there is no preference to know the absorption band of Manganese.

5.4 Experiment 3 - Interpretation of Functional Group

In experiment 3, degradation process cause the chages of the signal. Degradation due to the oxidation process as a result of exposing samples to the hot Manganese solution at 70°C for 1000 hours was detected by FTIR. Increase of the hot Mangnese solution exposure duration led to a significant increase in the carbonyl group concentration due to the higher oxidation of the molecules. Carbonyl groups usually account for most of the oxidation products on thermo-oxidative degradation of polyethylene; the concentration of carbonyl groups can be used to monitor the progress of degradation [15]. The carbonyl absorption is composed of different overlapping bands corresponding to acids, ketones , aldehydes and lactones. The presence of acids, ketones, aldehydes and lactones is depending on presence of other bands of functional groups such OH group and CO groups. The appearance of CO and OH at several band determine the presence of corresponding carbonyl group [16].

After spectrogram is run by GUI system, Figure 5.41, Figure 5.42 and Figure 5.43 shown the signal of the spectrogram. Table 5.31, Table 5.42 and Table 5.43 is the result of presence functional group after degradation process. Table 5.44 show the summarize of presence of functional group from Data 10 to Data 12.

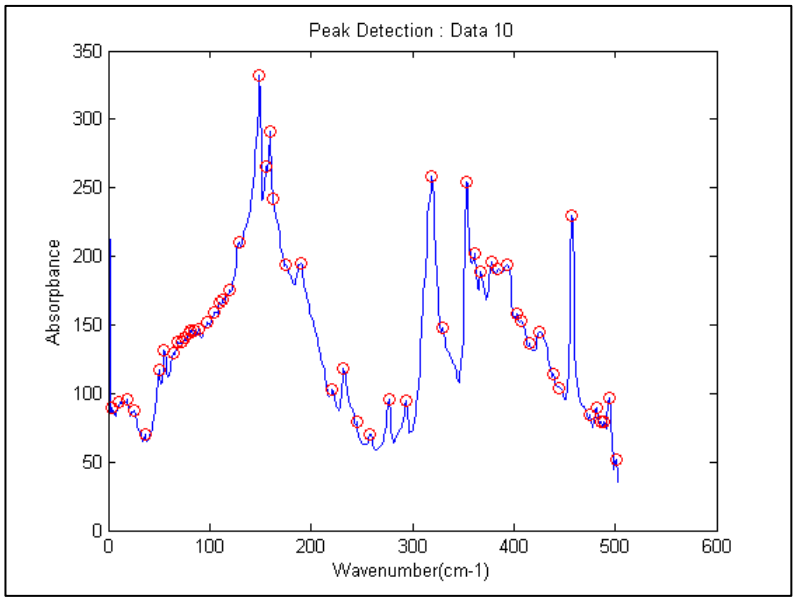


Figure 5.41: Signal of Data 10

Table 5.41 : Detection presence of Functional Group for Data 10

DATA 10			
Wavenumber cm^{-1}	Presence of Functional Group	Wavenumber cm^{-1}	Presence of Functional Group
4	0	221	0
11	0	232	0
19	0	245	0
25	0	258	0
36	0	277	0
50	0	294	0
55	0	319	C=O
64	0	330	C=O
69	0	353	0
72	0	361	0
75	0	367	0
79	0	378	0
81	0	384	0
85	0	393	CO
89	0	403	CO
98	0	407	CO
105	OH	415	CO
110	OH	425	CO
113	OH	439	VINYL
120	OH	445	0
129	OH	457	0
149	OH	475	0
156	OH	482	0
159	OH	486	0
163	OH	489	0
175	OH	494	0
190	OH		

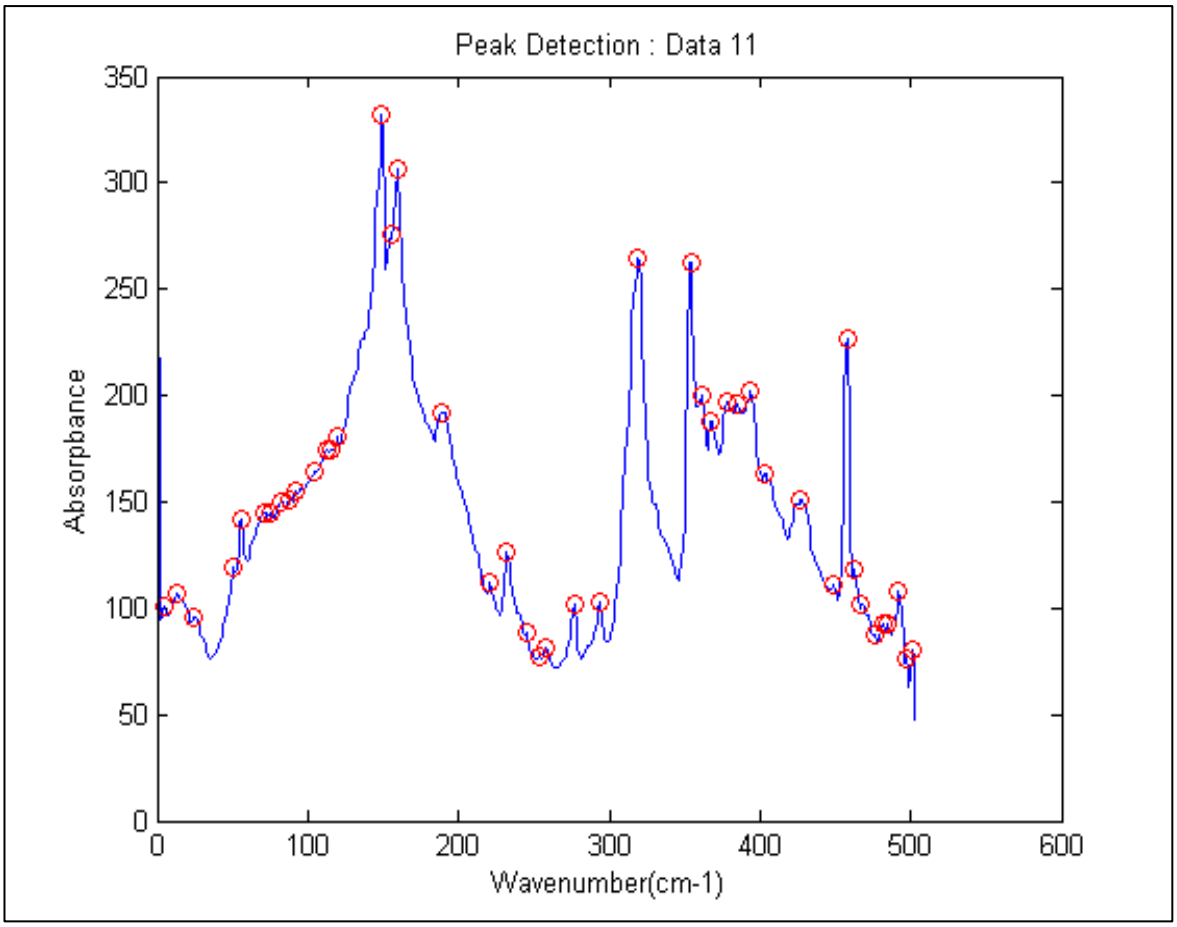


Figure 5.42: Signal of Data 11

Table 5.42 : Detection presence of Functional Group for Data 11

DATA 11			
Wavenumber cm^{-1}	Presence of Functional Group	Wavenumber cm^{-1}	Presence of Functional Group
5	0	253	0
13	0	258	0
24	0	277	0
51	0	294	0
56	0	319	C=O
71	0	354	0
75	0	361	0
82	0	367	0
88	0	378	0
92	0	385	0
104	OH	394	CO
112	OH	403	CO
115	OH	427	CO
119	OH	448	0
149	OH	458	0
155	OH	463	0
159	OH	467	0
189	OH	476	0
221	0	482	0
232	0	485	0
245	0	492	0
		497	0

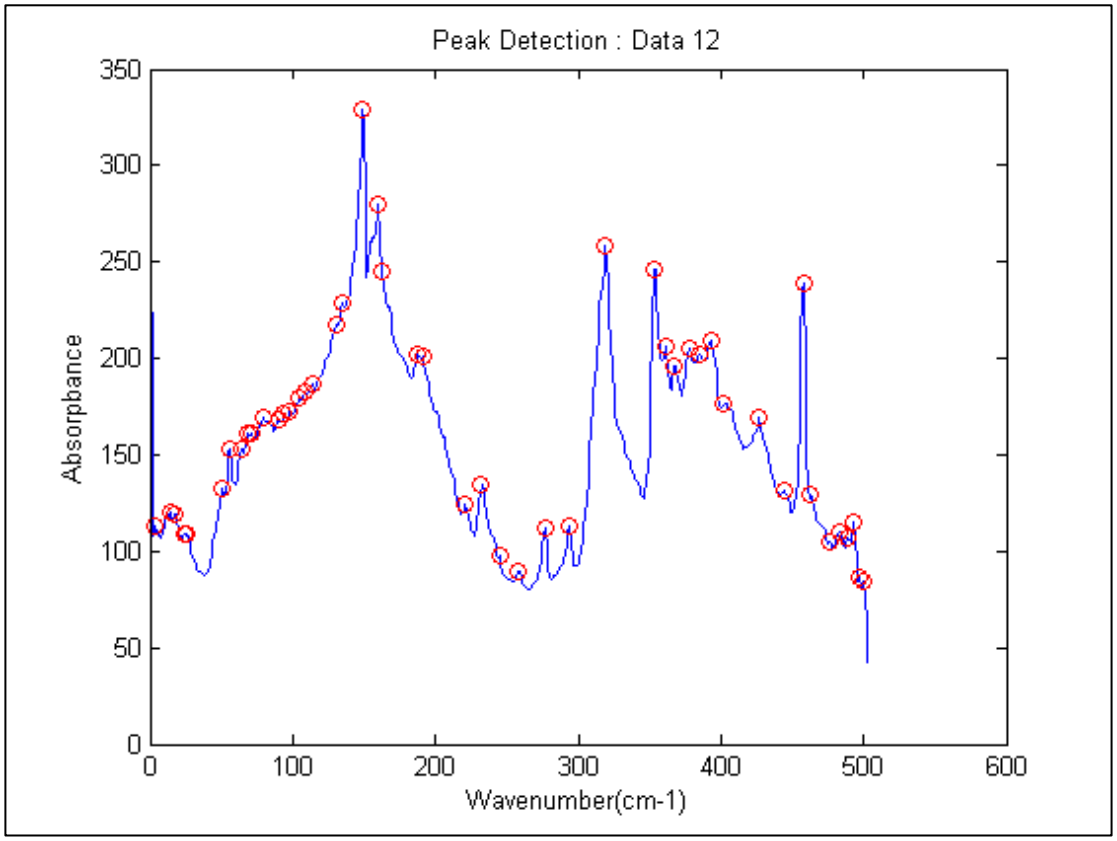


Figure 5.43: Signal of Data 12

Table 5.43 : Detection presence of Functional Group for Data 12

DATA 12			
Wavenumber cm^{-1}	Presence of Functional Group	Wavenumber cm^{-1}	Presence of Functional Group
4	0	221	0
14	0	232	0
17	0	245	0
24	0	258	0
26	0	277	0
51	0	294	0
56	0	319	C=O
64	0	353	0
69	0	361	0
71	0	367	0
79	0	378	0
90	0	385	0
94	0	393	CO
98	0	402	CO
105	OH	427	CO
109	OH	444	0
114	OH	458	0
130	OH	463	0
135	OH	476	0
149	OH	483	0
160	OH	489	0
163	OH	493	0
188	OH	497	0
191	OH	500	0

Table 5.43 : Detection presence of Functional Group for Data 10, Data 11 and Data 12

PRESENCE OF FUNCTIONAL GROUP	DATA 10 cm^{-1}	DATA 11 cm^{-1}	DATA12 cm^{-1}
OH	105	104	105
	110	112	109
	113	115	114
	120	119	130
	129	149	135
	149	155	149
	156	159	160
	159	189	163
	163	-	188
	175	-	191
	190	-	-
C=O	319	319	319
	330	-	-
CO	393	394	393
	403	403	402
	407	427	427
	415	-	-
	425	-	-
VINYL	439	-	-

From Table 5.43 the presence of OH group at Data 10 is started at band 105 cm^{-1} same as Data 12. At Data 11 OH group is presence at 104cm^{-1}. Result for Data 10 show that there are 11 of OH group presence. For Data 11 and 12, there are 8 and 10 of OH group presence respectively. Even though, the number of OH presence is different between the data, but all the data show the OH band is appear around 100cm^{-1} to 190cm^{-1}. The band for each data is not having many different between each other.

For example, for Data 10 and Data 12 detect the OH at 105cm^{-1}, else Data 2 detect OH group at 104cm^{-1}. Because there only once different, the appearance of OH at both band can be considered. In the conclusion, all the band of all data can be accepted to identify the presence of OH group in this chemical solution.

But there are some band need to be considered such in Data 10 at 175cm^{-1} and Data 12 at 135cm^{-1}. This consideration is made up because at band 175cm^{-1} only Data 10 presence this band. Data 11 and Data 12 did not have any band related to 170cm^{-1} to 179cm^{-1}. This analysis is same goes to Data 12, which only has value at 135cm^{-1}. Compared to Data 10 and Data 11, there is no value between 130cm^{-1} to 139cm^{-1}. Based in on this reason, all band from Data 10 to Data 12 can be accepted accept band 175cm^{-1} and 135cm^{-1} at Data 10 and Data 12 respectively.

For carbonyl group, C=O, all data shown the presence of this group at band 319cm^{-1}. In this solution, carbonyl group is presence at band 319cm^{-1}.

Analysis of CO group will be same as technique use to in OH group. All data show the presence of CO group in nearer band. Result shows that range of appearance CO group of data in range 393cm^{-1} to 427 cm^{-1}. In Data 10, appearance of CO group at 415cm^{-1} cannot be accepted as there is no band between 410cm^{-1} to 420cm^{-1} in Data 11 and Data 12. Vinyl group appear once in Data 10 at band 439cm^{-1}. Table 5.34 show the presence of Functional group and its corresponding band in this solution after some discussion has been made up.

Table 5.44: Presence of Functional Group in Polyethylene after degradation process

Presence of Functional Group	Wavenumber cm^{-1}	Presence of Functional Group	Wavenumber cm^{-1}
OH	104	C=O	319
	105		330
	109	CO	393
	110		394
	112		402
	113		403
	114		407
	115		425
	119		427
	120	VINYL	439
	129		
	130		
	149		
	155		
	156		
	159		
	160		
	163		
	188		
	189		
	190		
	191		

Refer to *library* in *Appendix A* and compare the band (wavenumber,cm^{-1}) to its corresponding band range. Table 5.45 show the result of comparison to corresponding band.

Table 5.45(a): Wavenumber of signal and its correspondent range

Functional Group	Wavenumber cm^{-1}	Corresponding Wavenumber cm^{-1}
OH	104	3285-3279
	105	3278-3272
	109	3250-3244
	110	3243-3237
	112	3229-3223
	113	3222-3216
	114	3215-3209
	115	3208-3202
	119	3180-3174
	120	3173-3167
	129	3110-3104
	130	3103-3097
	149	2970-2964
	155	2928-2922
	156	2921-2915
	159	2900-2894
	160	2893-2887
	163	2872-2866
	188	2697-2691
	189	2690-2684
	190	2684-2677
	191	2676-2670

Table 5.45(b): Wavenumber of signal and its correspondent range

Functional Group	Wavenumber cm^{-1}	Corresponding Wavenumber cm^{-1}
C=O	319	1780-1774
	330	1703-1697
CO	393	1262-1256
	394	1255-1249
	402	1199-1193
	403	1192-1186
	407	1164-1158
	425	1038-1032
	427	1024-1018
VINYL	439	940-934

Table 3.46: 'Fingerprint' Presence of Functional Group based on Band Range (Wavenumber, cm^{-1}) [19]

Wavenumber ,cm-1	Corresponding Band	Functional Group
3300-2500 cm^{-1}	ACID	O-H
1100-1300 cm^{-1}		C-O
1300-1000 cm^{-1}	ESTER	C-O
2850 cm^{-1} and 2750 cm^{-1}	ALDEHYDE	C-H
900-1000 cm^{-1}	-	VINYL
1600-1800cm^{-1}	CARBONYL	C=O

To prove the presence of the functional group in this project, compare the information in Table 3.45 and Table 3.46.

OH Group presence in this solution is in range 2670cm^{-1} – 3285cm^{-1}. As compare to range band of OH in Table 3.56 is around 3300cm^{-1} – 2500cm^{-1}. The result proves that functional group OH is presence. Functional group C=O in this project is appear around 1697cm^{-1} – 1780cm^{-1} as compare to Table 3.46, the presence of C=O is acceptable as the result in range 1800cm^{-1} – 1600cm^{-1}. According to Table 5.46, 1300cm^{-1} – 1000cm^{-1} is assign to functional group of CO. Compare to result for CO

group in this project, CO presence at 1262cm^{-1} – 1018cm^{-1}. It seems that CO also presence alongside with OH and C=O group. Vinyl group also can be approved it presence in this solution as it appear in range 900cm^{-1} – 1000cm^{-1}.

As a conclusion, after polyethylene undergo degradation process, there are presence of some functional group such OH, CO, C=O and Vinyl group in the solution. The presence of functional group in different region or band will help chemist related to chemical field.

CHAPTER 6

CONCLUSSION AND RECOMANDATION

As a conclusion here, functional group of HDPE is identified based on image of spectrogram. In experiment 1, the presence of CH_2 at band 164cm^{-1},386cm^{-1}, and CH_3 at band 149cm^{-1}, show that the fundamental of polyethylene. After degradation process in experiment 3, it show the presence of functional group such OH, CO, C=O and vinyl group at their corresponding band. This project also uses image processing as new approach to identify the functional group in HDPE.

The problem regarding this project is identifying the carbonyl group, C=O. C=O is composed with Ester, Aldehyde and Acid. In future research the other groups presence in C=O can be identify.

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Wavenumber cm^{-1}	Corresponding Wavenumber cm^{-1}	Range of Corresponding Wavenumber	Presence of CH Group	Presence of Functional Group
0	4000	4000	0	0
1	3993	3999-3993	0	0
2	3986	3994-3986	0	0
3	3979	3985-3979	0	0
4	3972	3978-3972	0	0
5	3965	3973-3966	0	0
6	3958	3965-3958	0	0
7	3951	3957-3951	0	0
8	3944	3950-3944	0	0
9	3937	3943-3937	0	0
10	3930	3936-3930	0	0
11	3923	3929-3923	0	0
12	3916	3922-3916	0	0
13	3909	3915-3909	0	0
14	3902	3908-3902	0	0
15	3895	3901-3895	0	0
16	3888	3894-3888	0	0
17	3881	3887-3881	0	0
18	3874	3880-3874	0	0
19	3867	3873-3867	0	0
20	3860	3866-3860	0	0
21	3853	3859-3853	0	0
22	3846	3852-3846	0	0
23	3839	3845-3839	0	0
24	3832	3828-3832	0	0
25	3825	3831-3825	0	0
26	3818	3824-3818	0	0
27	3811	3817-3811	0	0
28	3804	3819-3804	0	0
29	3797	3803-3797	0	0
30	3790	3796-3790	0	0
31	3783	3789-3783	0	0
32	3776	3782-3776	0	0
33	3769	3775-3769	0	0
34	3762	3768-3762	0	0
35	3755	3761-3755	0	0

0=none of functional or CH group presence,
2=CH_2,3=CH_3,11=OH,12=CO,13=CH,14=Vinyl,15=C=O

Wavenumber cm^{-1}	Corresponding Wavenumber cm^{-1}	Range of Corresponding Wavenumber	Presence of CH Group	Presence of Functional Group
36	3748	3754-3748	0	0
37	3741	3747-3741	0	0
38	3734	3740-3734	0	0
39	3727	37323-3727	0	0
40	3720	3726-3720	0	0
41	3713	3719-3713	0	0
42	3706	3712-3706	0	0
43	3699	3705-3699	0	0
44	3692	3698-3692	0	0
45	3685	3691-3685	0	0
46	3678	3684-3678	0	0
47	3671	3677-3671	0	0
48	3664	3670-3664	0	0
49	3657	3663-3657	0	0
50	3650	3656-3650	0	0
51	3643	3649-3643	0	0
52	3636	3642-3636	0	0
53	3629	3635-3629	0	0
54	3622	3628-3622	0	0
55	3615	3621-3615	0	0
56	3608	3614-3608	0	0
57	3601	3607-3601	0	0
58	3594	3600-3594	0	0
59	3587	3593-3587	0	0
60	3580	3586-3580	0	0
61	3573	3579-3573	0	0
62	3566	3572-3566	0	0
63	3559	3565-3559	0	0
64	3552	3558-3552	0	0
65	3545	3551-3545	0	0
66	3538	3544-3538	0	0
67	3531	3537-3531	0	0
68	3524	3530-3524	0	0
69	3517	3523-3517	0	0
70	3510	3516-3510	0	0
71	3503	3509-3503	0	0
72	3496	3502-3496	0	0

0=none of functional or CH group presence,
2=CH_2,3=CH_3,11=OH,12=CO,13=CH,14=Vinyl,15=C=O

Wavenumber cm^{-1}	Corresponding Wavenumber cm^{-1}	Range of Corresponding Wavenumber	Presence of CH Group	Presence of Functional Group
73	3489	3495-3489	0	0
74	3482	3488-3482	0	0
75	3475	3481-3475	0	0
76	3468	3474-3468	0	0
77	3461	3467-3461	0	0
78	3454	3460-3454	0	0
79	3447	3453-2447	0	0
80	3440	3446-3440	0	0
81	3433	3439-3433	0	0
82	3426	3432-3426	0	0
83	3419	3425-3419	0	0
84	3412	3418-3412	0	0
85	3405	3411-3405	0	0
86	3398	3404-3398	0	0
87	3391	3397-3391	0	0
88	3384	3390-3384	0	0
89	3377	3383-3377	0	0
90	3370	3376-3370	0	0
91	3363	3366-3363	0	0
92	3356	3362-3356	0	0
93	3349	3355-3349	0	0
94	3342	3348-3342	0	0
95	3335	3341-3335	0	0
96	3328	3334-3328	0	0
97	3321	3327-3321	0	0
98	3314	3320-3314	0	0
99	3307	3315-3307	0	0
100	3300	3306-3300	0	11
101	3293	3299-3293	0	11
102	3286	3291-3286	0	11
103	3279	3285-3279	0	11
104	3272	3278-3272	0	11
105	3265	3271-3265	0	11
106	3258	3264-3258	0	11
107	3251	3257-3251	0	11
108	3244	3250-3244	0	11
109	3237	3243-3237	0	11

0=none of functional or CH group presence,
2=CH_2,3=CH_3,11=OH,12=CO,13=CH,14=Vinyl,15=C=O

Wavenumber cm^{-1}	Corresponding Wavenumber cm^{-1}	Range of Corresponding Wavenumber	Presence of CH Group	Presence of Functional Group
110	3230	3236-3230	0	11
111	3223	3229-3223	0	11
112	3216	3222-3216	0	11
113	3209	3215-3209	0	11
114	3202	3208-3202	0	11
115	3195	3201-3195	0	11
116	3188	3194-3188	0	11
117	3181	3187-3181	0	11
118	3174	3180-3174	0	11
119	3167	3173-3167	0	11
120	3160	3166-3160	0	11
121	3153	3159-3153	0	11
122	3146	3152-3146	0	11
123	3139	3145-3139	0	11
124	3132	3138-3132	0	11
125	3125	3131-3125	0	11
126	3118	3124-3118	0	11
127	3111	3117-3111	0	11
128	3104	3110-3104	0	11
129	3097	3103-3097	0	11
130	3090	3096-3090	0	11
131	3083	3089-3083	0	11
132	3076	3082-3076	0	11
133	3069	3075-3069	0	11
134	3062	3068-3062	0	11
135	3055	3061-3055	0	11
136	3048	3054-3048	0	11
137	3041	3047-3041	0	11
138	3034	3040-3034	0	11
139	3027	3-33-3027	0	11
140	3020	3026-3020	0	11
141	3013	3019-3013	0	11
142	3006	3012-3006	0	11
143	2999	3005-2999	0	11
144	2992	2998-3992	0	11
145	2985	3991-3985	0	11
146	2978	3984-2978	0	11

0=none of functional or CH group presence,
2=CH_2,3=CH_3,11=OH,12=CO,13=CH,14=Vinyl,15=C=O

Wavenumber cm^{-1}	Corresponding Wavenumber cm^{-1}	Range of Corresponding Wavenumber	Presence of CH Group	Presence of Functional Group
147	2971	2977-2971	0	11
148	2964	2970-2964	0	11
149	2957	2963-2957	3	11
150	2950	2956-2950	0	11
151	2943	2949-2943	0	11
152	2936	2942-2936	0	11
153	2929	2935-2929	0	11
154	2922	2928-2922	2	11
155	2915	2921-2915	0	11
156	2908	2914-2908	0	11
157	2901	2907-2901	0	11
158	2894	2900-2894	0	11
159	2887	2893-2887	0	11
160	2880	2886-2880	0	11
161	2873	2879-2873	3	11
162	2866	2872-2866	0	11
163	2859	2865-2869	2	11
164	2852	2858-2852	2	11
165	2845	2851-3845	0	13
166	2838	2844-2838	0	11
167	2831	2837-2831	0	11
168	2824	3830-2824	0	11
169	2817	2823-2817	0	11
170	2810	2816-2810	0	11
171	2803	2809-2803	0	11
172	2796	2802-2796	0	11
173	2789	2795-2789	0	11
174	2782	2788-2782	0	11
175	2775	2781-2775	0	11
176	2768	2774-2768	0	11
177	2761	2767-2761	0	11
178	2754	2760-2754	0	13
179	2747	2753-2747	0	11
180	2740	2746-2740	0	11
181	2733	2739-2733	0	11
182	2726	2732-2726	0	11
183	2719	3725-2719	0	11

0=none of functional or CH group presence,
2=CH_2,3=CH_3,11=OH,12=CO,13=CH,14=Vinyl,15=C=O

Wavenumber cm^{-1}	Corresponding Wavenumber cm^{-1}	Range of Corresponding Wavenumber	Presence of CH Group	Presence of Functional Group
184	2712	2718-2712	0	11
185	2705	2711-2705	0	11
186	2698	2704-2698	0	11
187	2691	2697-2691	0	11
188	2684	2690-2684	0	11
189	2677	2684-2677	0	11
190	2670	2676-2670	0	11
191	2663	2669-2663	0	11
192	2656	2662-2656	0	11
193	2649	2655-2649	0	11
194	2642	2648-2642	0	11
195	2635	2641-3635	0	11
196	2628	2634-262	0	11
197	2621	2627-2621	0	11
198	2614	2620-2614	0	11
199	2607	2613-2607	0	11
200	2600	2608-2600	0	11
201	2593	2599-2593	0	11
202	2586	2592-2586	0	11
203	2579	2585-2579	0	11
204	2572	2578-2572	0	11
205	2565	2571-2565	0	11
206	2558	2565-2558	0	11
207	2551	2557-2551	0	11
208	2544	2550-2544	0	11
209	2537	2543-2537	0	11
210	2530	2536-2530	0	11
211	2523	2529-2523	0	11
212	2516	2522-2516	0	11
213	2509	2515-2509	0	11
214	2502	2508-2502	0	11
215	2495	2501-2495	0	11
216	2488	2494-2488	0	0
217	2481	2487-2481	0	0
218	2474	2480-2474	0	0
219	2467	2473-2467	0	0
220	2460	2465-2460	0	0

0=none of functional or CH group presence,
2=CH_2,3=CH_3,11=OH,12=CO,13=CH,14=Vinyl,15=C=O

Wavenumber cm^{-1}	Corresponding Wavenumber cm^{-1}	Range of Corresponding Wavenumber	Presence of CH Group	Presence of Functional Group
221	2453	2459-2453	0	0
222	2446	2452-2446	0	0
223	2439	2445-2439	0	0
224	2432	2438-2432	0	0
225	2425	2431-2424	0	0
226	2418	2424-2418	0	0
227	2411	2417-2411	0	0
228	2404	2410-2404	0	0
229	2397	2403-2397	0	0
230	2390	2396-2390	0	0
231	2383	2389-2383	0	0
232	2376	2382-2376	0	0
233	2369	2375-2369	0	0
234	2362	2368-2362	0	0
235	2355	2361-2355	0	0
236	2348	2354-2348	0	0
237	2341	2347-2341	0	0
238	2334	2340-2334	0	0
239	2327	2333-2327	0	0
240	2320	2326-2320	0	0
241	2313	2319-2313	0	0
242	2306	2312-2306	0	0
243	2299	2305-2299	0	0
244	2292	2298-2292	0	0
245	2285	2291-2285	0	0
246	2278	2284-2278	0	0
247	2271	2277-2271	0	0
248	2264	2270-2264	0	0
249	2257	2263-2257	0	0
250	2250	2256-2250	0	0
251	2243	2249-2243	0	0
252	2236	2242-2236	0	0
253	2229	2237-2229	0	0
254	2222	2228-2222	0	0
255	2215	2221-2215	0	0
256	2208	2214-2208	0	0
257	2201	2207-2201	0	0

0=none of functional or CH group presence,
2=CH_2,3=CH_3,11=OH,12=CO,13=CH,14=Vinyl,15=C=O

Wavenumber cm^{-1}	Corresponding Wavenumber cm^{-1}	Range of Corresponding Wavenumber	Presence of CH Group	Presence of Functional Group
258	2194	2220-2194	0	0
259	2187	2193-2187	0	0
260	2180	2186-2180	0	0
261	2173	2179-2173	0	0
262	2166	2172-2166	0	0
263	2159	2165-2159	0	0
264	2152	2158-2152	0	0
265	2145	2151-2145	0	0
266	2138	2144-2138	0	0
267	2131	2137-2131	0	0
268	2124	2130-2124	0	0
269	2117	2123-2117	0	0
270	2110	2116-2110	0	0
271	2103	2109=2103	0	0
272	2096	2102-2096	0	0
273	2089	2097-2089	0	0
274	2082	2087-2082	0	0
275	2075	2081-2075	0	0
276	2068	2074-2068	0	0
277	2061	2067-2061	0	0
278	2054	2060-2054	0	0
279	2047	2053-2047	0	0
280	2040	2046-2040	0	0
281	2033	2039-2033	0	0
282	2026	2032-2026	0	0
283	2019	2025-2019	0	0
284	2012	2018-2012	0	0
285	2005	2011-2005	0	0
286	1998	2004-1998	0	0
287	1991	1997-1991	0	0
288	1984	1990-1984	0	0
289	1977	1983-1997	0	0
290	1970	1996-1970	0	0
291	1963	1969-1963	0	0
292	1956	1962-1956	0	0
293	1949	1955-1949	0	0
294	1942	1948-1942	0	0

0=none of functional or CH group presence,
2=CH_2,3=CH_3,11=OH,12=CO,13=CH,14=Vinyl,15=C=O

Wavenumber cm^{-1}	Corresponding Wavenumber cm^{-1}	Range of Corresponding Wavenumber	Presence of CH Group	Presence of Functional Group
295	1935	1941-1935	0	0
296	1928	1934-1928	0	0
297	1921	1937-1921	0	0
298	1914	1920-1914	0	0
299	1907	1913-1907	0	0
300	1900	1906-1900	0	0
301	1893	1899-1893	0	0
302	1886	1892-1886	0	0
303	1879	1887-1879	0	0
304	1872	1878-1872	0	0
305	1865	1871-1865	0	0
306	1858	1864-1858	0	0
307	1851	1857-1851	0	0
308	1844	1850-1844	0	0
309	1837	1843-1837	0	0
310	1830	1836-1830	0	0
311	1823	1839-1823	0	0
312	1816	1822-1816	0	0
313	1809	1815-1809	0	0
314	1802	1808-1802	0	0
315	1795	1801-1795	0	15
316	1788	1794-1788	0	15
317	1781	1787-1781	0	15
318	1774	1780-1774	0	15
319	1767	1773-1767	0	15
320	1760	1766-1760	0	15
321	1753	1759-1753	0	15
322	1746	1752-1746	0	15
323	1739	1745-1739	0	15
324	1732	1738-1732	0	15
325	1725	1731-1725	0	15
326	1718	1724-1718	0	15
327	1711	1717-1711	0	15
328	1704	1710-1704	0	15
329	1697	1703-1697	0	15
330	1690	1696-1690	0	15
331	1683	1689-1683	0	15

0=none of functional or CH group presence,
2=CH_2,3=CH_3,11=OH,12=CO,13=CH,14=Vinyl,15=C=O

Wavenumber cm^{-1}	Corresponding Wavenumber cm^{-1}	Range of Corresponding Wavenumber	Presence of CH Group	Presence of Functional Group
295	1935	1941-1935	0	0
332	1676	1682-1676	0	15
333	1669	1675-1669	0	15
334	1662	1668-1662	0	15
335	1655	1661-1655	0	15
336	1648	1654-1648	0	15
337	1641	1647-1641	0	15
338	1634	1640-1634	0	15
339	1627	1633-1627	0	15
340	1620	1626-1620	0	15
341	1613	1619-1613	0	15
342	1606	1612-1606	0	15
343	1599	1605-1599	0	15
344	1592	1598-1592	0	0
345	1585	1591-1585	0	0
346	1578	1584-1578	0	0
347	1571	1577-1571	0	0
348	1564	1570-1564	0	0
349	1557	1563-1557	0	0
350	1550	1556-1550	0	0
351	1543	1549-1543	0	0
352	1536	1542-1536	0	0
353	1529	1535-1529	0	0
354	1522	1528-1522	0	0
355	1515	1521-1515	0	0
356	1508	1514-1508	0	0
357	1501	1507-1501	0	0
358	1494	1500-1494	0	0
359	1487	1493-1487	0	0
360	1480	1486-1480	0	0
361	1473	1479-1473	0	0
362	1466	1472-1466	2	0
363	1459	1465-1459	3	0
364	1452	1458-1452	3	0
365	1445	1451-1445	0	0
366	1438	1444-1438	0	0
367	1431	1437-1431	0	0

0=none of functional or CH group presence,
2=CH_2,3=CH_3,11=OH,12=CO,13=CH,14=Vinyl,15=C=O

Wavenumber cm^{-1}	Corresponding Wavenumber cm^{-1}	Range of Corresponding Wavenumber	Presence of CH Group	Presence of Functional Group
369	1417	1423-1417	0	0
370	1410	1416-1410	0	0
371	1403	1409-1403	0	0
372	1396	1402-1396	0	0
373	1389	1395-1389	0	0
374	1382	1388-1382	0	0
375	1375	1381-1375	3	0
376	1368	1374-1368	2	0
377	1361	1367-1361	0	0
378	1354	1360-1354	0	0
379	1347	1353-1347	2	0
380	1340	1346-1340	0	0
381	1333	1339-1333	0	0
382	1326	1332-1326	0	0
383	1319	1325-1319	0	0
384	1312	1318-1312	0	0
385	1305	1311-1305	0	0
386	1298	1304-1298	2	12
387	1291	1297-1291	0	12
388	1284	1290-1284	0	12
389	1277	1283-1277	0	12
390	1270	1276-1270	0	12
391	1263	1269-1263	0	12
392	1256	1262-1256	0	12
393	1249	1255-1249	0	12
394	1242	1248-1242	0	12
395	1235	1241-1235	0	12
396	1228	1234-1228	0	12
397	1221	1227-1221	0	12
398	1214	1220-1214	0	12
399	1207	1213-1207	0	12
400	1200	1206-1200	0	12
401	1193	1199-1193	0	12
402	1186	1192-1186	0	12
403	1179	1185-1179	0	12
404	1172	1178-1172	0	12
405	1165	1171-1165	0	12

0=none of functional or CH group presence,
2=CH_2,3=CH_3,11=OH,12=CO,13=CH,14=Vinyl,15=C=O

Wavenumber cm^{-1}	Corresponding Wavenumber cm^{-1}	Range of Corresponding Wavenumber	Presence of CH Group	Presence of Functional Group
406	1158	1164-1158	0	12
407	1151	1157-1151	0	12
408	1144	1150-1144	0	12
409	1137	1143-1137	0	12
410	1130	1136-1130	0	12
411	1123	1129-1123	0	12
412	1116	1122-1116	0	12
413	1109	1115-1109	0	12
414	1102	1108-1102	0	12
415	1095	1101-1095	0	12
416	1088	1094-1088	0	12
417	1081	1087-1081	0	12
418	1074	1080-1074	0	12
419	1067	1073-1067	0	12
420	1060	1065-1060	0	12
421	1053	1059-1053	0	12
422	1046	1052-1046	0	12
423	1039	1045-1039	0	12
424	1032	1038-1032	0	12
425	1025	1031-1025	0	12
426	1018	1024-1018	0	12
427	1011	1017-1011	0	12
428	1004	1010-1004	0	12
429	997	1003-997	0	12
430	990	996-990	0	14
431	983	989-983	0	14
432	976	982-976	0	14
433	969	975-969	0	14
434	962	968-962	0	14
435	955	961-955	0	14
436	948	954-948	0	14
437	941	9447-941	0	14
438	934	940-934	0	14
439	927	933-927	0	14
440	920	926-920	0	14
441	913	919-913	0	14
442	906	912-906	0	14

0=none of functional or CH group presence,
2=CH_2,3=CH_3,11=OH,12=CO,13=CH,14=Vinyl,15=C=O

Wavenumber cm^{-1}	Corresponding Wavenumber cm^{-1}	Range of Corresponding Wavenumber	Presence of CH Group	Presence of Functional Group
443	899	905-899	0	14
444	892	898-892	0	0
445	885	891-885	3	0
446	878	884-878	0	0
447	871	877-871	0	0
448	864	870-864	0	0
449	857	863-857	0	0
450	850	856-850	0	0
451	843	849-843	0	0
452	836	842-836	0	0
453	829	835-829	0	0
454	822	828-822	0	0
455	815	821-815	0	0
456	808	814-808	0	0
457	801	807-801	0	0
458	794	800-794	0	0
459	787	793-787	0	0
460	780	786-780	0	0
461	773	779-773	0	0
462	766	772-766	0	0
463	759	765-759	0	0
464	752	758-752	0	0
465	745	751-745	0	0
466	738	744-738	0	0
467	731	737-731	2	0
468	724	730-724	2	0
469	717	723-717	0	0
470	710	716-710	0	0
471	703	709-703	0	0
472	696	702-696	0	0
473	689	695-689	0	0
474	682	688-682	0	0
475	675	681-675	0	0
476	668	674-668	0	0
477	661	667-661	0	0
478	654	660-654	0	0
479	647	653-647	0	0

0=none of functional or CH group presence,
2=CH_2,3=CH_3,11=OH,12=CO,13=CH,14=Vinyl,15=C=O

Wavenumber cm^{-1}	Corresponding Wavenumber cm^{-1}	Range of Corresponding Wavenumber	Presence of CH Group	Presence of Functional Group
480	640	646-640	0	0
481	633	639-633	0	0
482	626	632-626	0	0
483	619	627-619	0	0
484	612	618-612	0	0
485	605	611-605	0	0
486	598	604-598	0	0
487	591	597-591	0	0
488	584	590-584	0	0
489	577	583-577	0	0
490	570	576-570	0	0
491	563	569-563	0	0
492	556	562-556	0	0
493	549	555-549	0	0
494	542	458-542	0	0
495	535	541-535	0	0
496	528	534-528	0	0
497	521	527-521	0	0
498	514	520-514	0	0
499	507	513-507	0	0
500	500	506-500	0	0

0=none of functional or CH group presence,
2=CH_2,3=CH_3,11=OH,12=CO,13=CH,14=Vinyl,15=C=O