

# The $^1\text{H}$ and $^{13}\text{C}$ NMR Spectra for Poly methylmethacrylate before and after exposure to the MRI Field

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**ABSTRACT:** This particular research study influence and effects of MRI field on spectra analysis for  $^1\text{H}$  and  $^{13}\text{C}$  of Poly methylmethacrylate and comparing this effects before and after exposure to (MRI) field. The results showed that comparing chart for  $^1\text{H}$  and  $^{13}\text{C}$  analysis for different samples of Polymethyl-methacrylate Pink and clean, no significant for differences have been found yet.

**Keywords:** (MRI) wave,  $^1\text{H}$ NMR,  $^{13}\text{C}$  NMR, Poly methyl methacrylate.

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## INTRODUCTION

### Polymethyl- methacrylate properties and characteristics

Polymethyl- methacrylate is an essential part of what called acyclic- plastic, which has been supplied in a variety of forms like powder gel, sheets, contains many additives like clear, pigmented, characters, plastic fibers. <sup>(1)</sup>. Polymethyl-methacrylate compose of small spheres beads or pearls and peroxide exist to initiate reaction depend on way of decomposition happened, and contain titanium dioxide in small amount for opacity and inorganic material like mercuric sulfide (red), cadmium sulfide (yellow), ferric oxide to match color wanted to be gained, with dyed Symantec fiber to simulate the minute blood- vessels. <sup>(2)(3)</sup>

### Polymethyl methacrylate

Generally polymethyl methacrylate have low thermal conductivity, with heat distortion temperature relatively low, 95°C volumetric polymerization shrinkage of a 3:1 ratio with possibility of 2% of linear shrinkage, adhesion to metal and porcelain is poor and bonding is only accomplished by mechanical retention and a compound called (4 META) (4-methacryloxyethyl tri-mellitus anhydride) when present at ratio (10-15%) increase adhesive properties and this polymer usually with color stability good and with law risk of toxicity or allergic reaction. <sup>(4)</sup>

### Magnetic Resonances Imaging Field (MRI)

#### Magnetic Resonance Image (MRI) Definition

MRI is device for high resolution image used for viewing stricture, and it is basic principle depend on exists of hydrogen atoms nucleus subjected to high powerful magnetic lead to hydrogen atoms to be aligned in certain forms <sup>(15)(5)</sup>.

#### (MRI) principles and practice

The routine (MRI) depend on exist of "H" atom inside any material under study and when subjected to high magnetic fields (e.g., 1 tesla = 100000 gauss) the small nuclei act like tiny magnetic make up <sup>(6)</sup>. Three-principle parameters of (MRI) including proton density which measure the concentration of mobile hydrogen nuclei available to produce on (MRI) signal <sup>(7)</sup>. And "T<sub>1</sub>" and "T<sub>2</sub>" relaxation time which the rate at which the used magnetization is to be return to the equilibrium state after pass through an abject or diseased tissue since "T<sub>1</sub>" is longitudinal relaxation and "T<sub>2</sub>" is a transverse relaxation <sup>(8)</sup>.

## Polymer interact with (MRI) wave

Based on principle that most of dental polymer and mainly "polymethyl methacrylate" contain an certain degree of different component like H, C, O<sub>2</sub>, S an increase interest now is growing to study this effect on (MRI) wave and study basic principle of polymer decomposition and analytic study <sup>(9)</sup>. And by studying all polymer like polymethyl methacrylate component and it is degreed interaction with magnetic field applied upon it, we can determined weather exposure to (MRI) field for period of time can change this polymer component ratio which eventually result in change polymer itself or it will pass though field of (MRI) and remain unchanged <sup>(10)</sup>.

### <sup>1</sup>H and <sup>13</sup>C NMR Spectroscopy:

#### NMR Spectroscopy: Act and Principle:

Nuclear magnetic resonance (NMR) deals mainly with atomic nuclei spin, since it contain a protons and neutrons with positive and negative charge <sup>(11)</sup>. And thus, when nuclei of an atom when exposed to an external magnetic field it will become by itself tiny magnetic, that it will line itself with an external magnetic field and making it is own gyroscopic spinning to compare it other spinning nuclei and to make an account indentation <sup>(12)</sup>. This makes (NMR) spectroscopy an invaluable tool for studying suitable changes in the distribution of electron density interaction between molecules and their environment interaction with the solvent and interaction inside of crystal have long been under investigation <sup>(13)</sup>.

By combination of a large dispersion of chemical shifts 1000 ppm for organic molecules and sensitivity to electronic interaction with <sup>13</sup>C interaction with existing of hydrogen H<sup>1</sup> atoms existing to make this tool is very sensitive probe for both structural changes and inter molecules interaction in hydrogen bonding studies especially in solutions and degree with rates of exchanges of proton transfer, the nature of the hydrogen bonds can be assessed by using <sup>1</sup>H and <sup>15</sup>N chemical shifts and indirect <sup>1</sup>H – <sup>15</sup>N coupling constants <sup>(13)</sup>. The aim of this study is to showed the effects of "MRI" waves on the structure of the poly methyl methacrylate by measuring the H<sup>1</sup> and C<sup>13</sup> spectroscopy, before and after exposure, thus evaluate possibility of any changes can been noticed as a result to exposer to (MRI) on different level.

#### Experiment Design and Work

\* (NMR) device: (NMR)-600 device is used for present study and this device carried out in (Colorado State University) USA.

\* Polymethyl-methacrylate: Two types of the Polymethyl methacrylate used is the study pink and clear and mixed type.

\* (MRI) Device:

An MRI device is used to provide a wave to expose all part of polymethyl methacrylate particles and For-adequate period of time to ensure exposure to (MRI) wave.

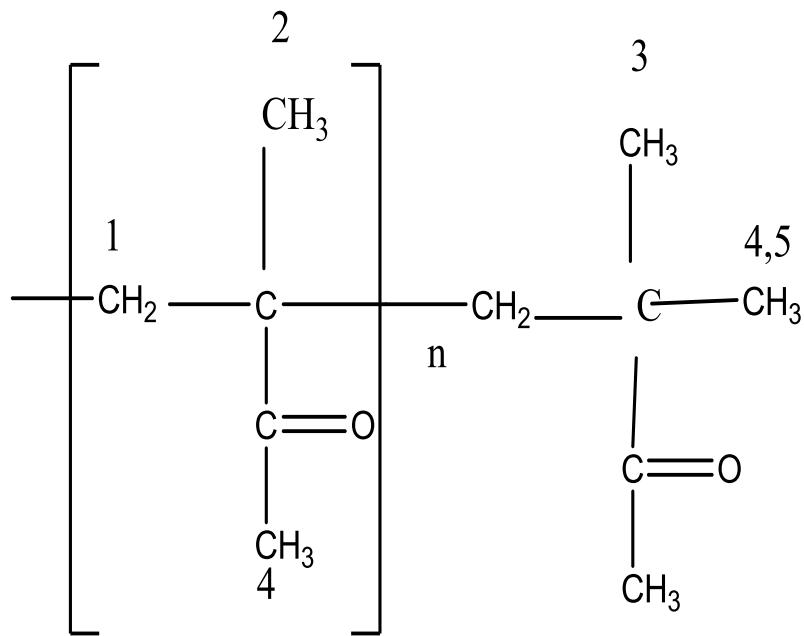
#### Samples Testing

The polymethyl methacrylate is prepared in the form of a powder and this powder must be diluted in a solution with an adequate degree of solvent which contain no hydrogen or carbon atoms of its on, it is mainly known as (carbon tetrachloride, deterred chloroform CDCl<sub>3</sub>) <sup>(14)</sup>. And then samples will places into (NMR) device, the device will work on re lax-delay time on 1.000 sec. and pulse on 45.degrees acquisition time on 1.285 sec. as an average time and degree of Hertz on 38 dB and on total time of testing through all the experiment on 38 min. Nuclear magnetic resonance spectroscopy (NMR): the measurement of NMR spectra were done at the Colorado State University (CSU). The structure of PMMA before and after exposure to MRI radiation was determined by NMR analysis. Proton NMR spectroscopy (HNMR): <sup>1</sup>HNMR spectra were measured on a Varia 400MHz instrument using CDCl<sub>3</sub> as solvent. All spectra were referenced to tetra methyl saline (TMS) at 0 ppm. Carbon NMR (<sup>13</sup>C NMR): <sup>13</sup> C NMR spectra were determined in the same manner as the proton <sup>1</sup>HNMR spectra. Nuclear magnetic resonance spectroscopy (NMR): the measurement of NMR spectra were done at the Colorado State University (CSU). The structure of PMMA before and after exposure to MRI radiation was determined by NMR analysis. Proton NMR spectroscopy (HNMR) : HNMR spectra were measured on a Varia 400MHz instrument using CDCl<sub>3</sub> as solvent. All spectra were referenced to tetra methyl saline (TMS) at 0 ppm. Carbon NMR (<sup>13</sup>C NMR): <sup>13</sup> C NMR spectra were determined in the same manner as the proton HNMR spectra.

#### RESULTS:

<sup>1</sup>HNMR analysis was carried out to confirm the structure of the poly methylmetacrylate before and after exposure to the MRI radiation.

HNMR spectra are shown in figures (1-3). The spectral data of PMMA before and after exposure are summarized in table 1. The structure of the PMMA can be illustrate by the following structure



**Table 1:  $^1\text{H}$ NMR data for PMMA before and after exposure**

$^1\text{H}$ NMR of PMMA	NMR shift (ppm) Before	NMR shift (ppm) After
H(1)	1.62	1.63
H(2)	0.97	0.97
H(3)	1.80	1.81
H(4)	3.57	3.57
H(5)	0.77	0.77

**Table 2:  $^{13}\text{C}$  NMR of PMMA before and after exposure**

$^{13}\text{C}$ NMR of PMMA	NMR shift (ppm) Before	NMR shift (ppm) After
C(1)	54.30	54.30
C(2)	19.00	19.00
C(3)	44.86	44.86
C(4)	178.33	178.33
C(5)	52.10	52.10
C(6)	17.08	17.08

### $^{13}\text{C}$ NMR analysis

$^{13}\text{C}$  NMR analysis was also used to confirm if there are any change in the structure before and after exposure PMMA to MRI.

$^{13}\text{C}$  NMR spectra before and after exposure are shown in figures (4-6). The spectral data are summarized in table 1 and 2

## Results

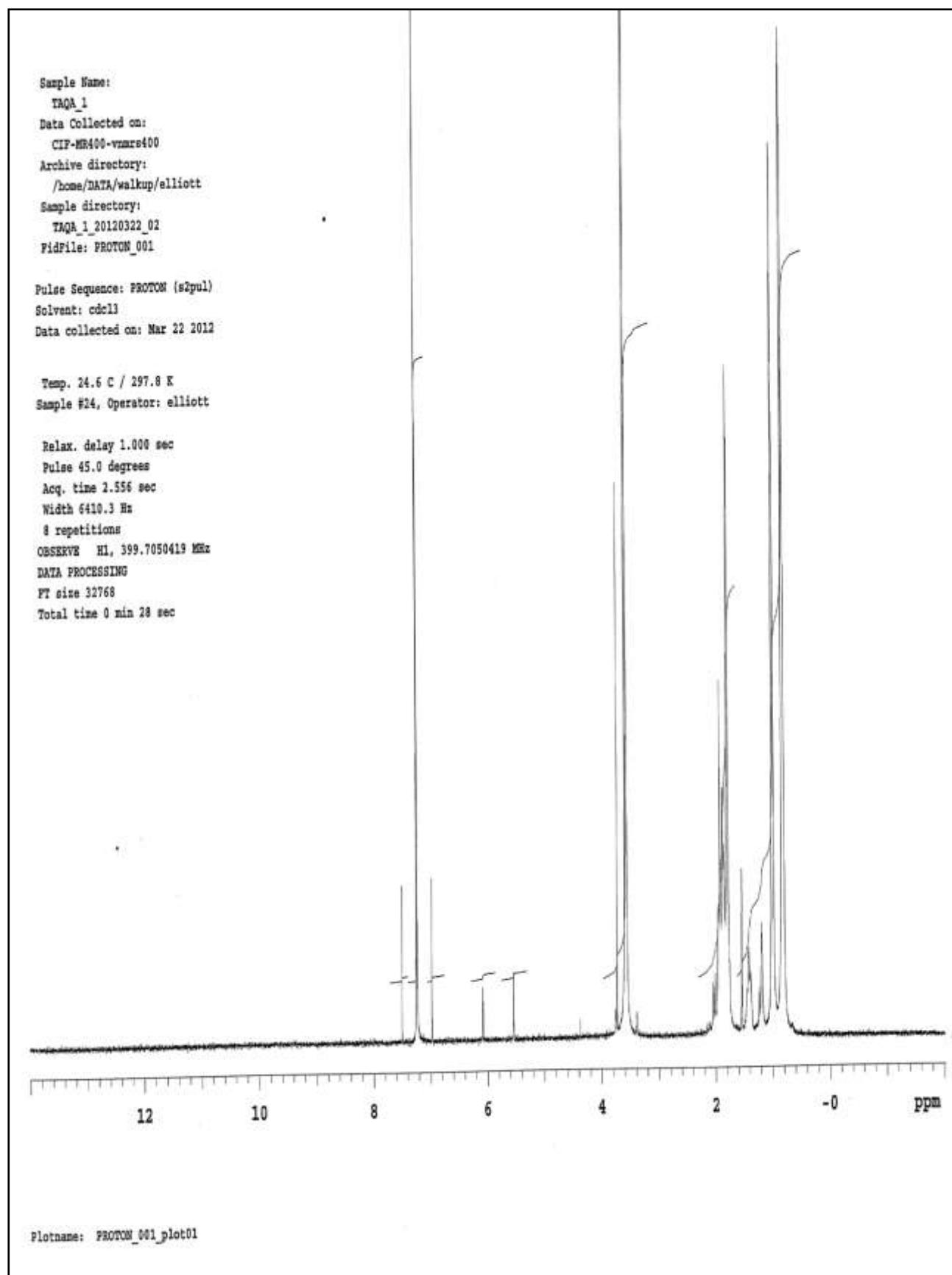
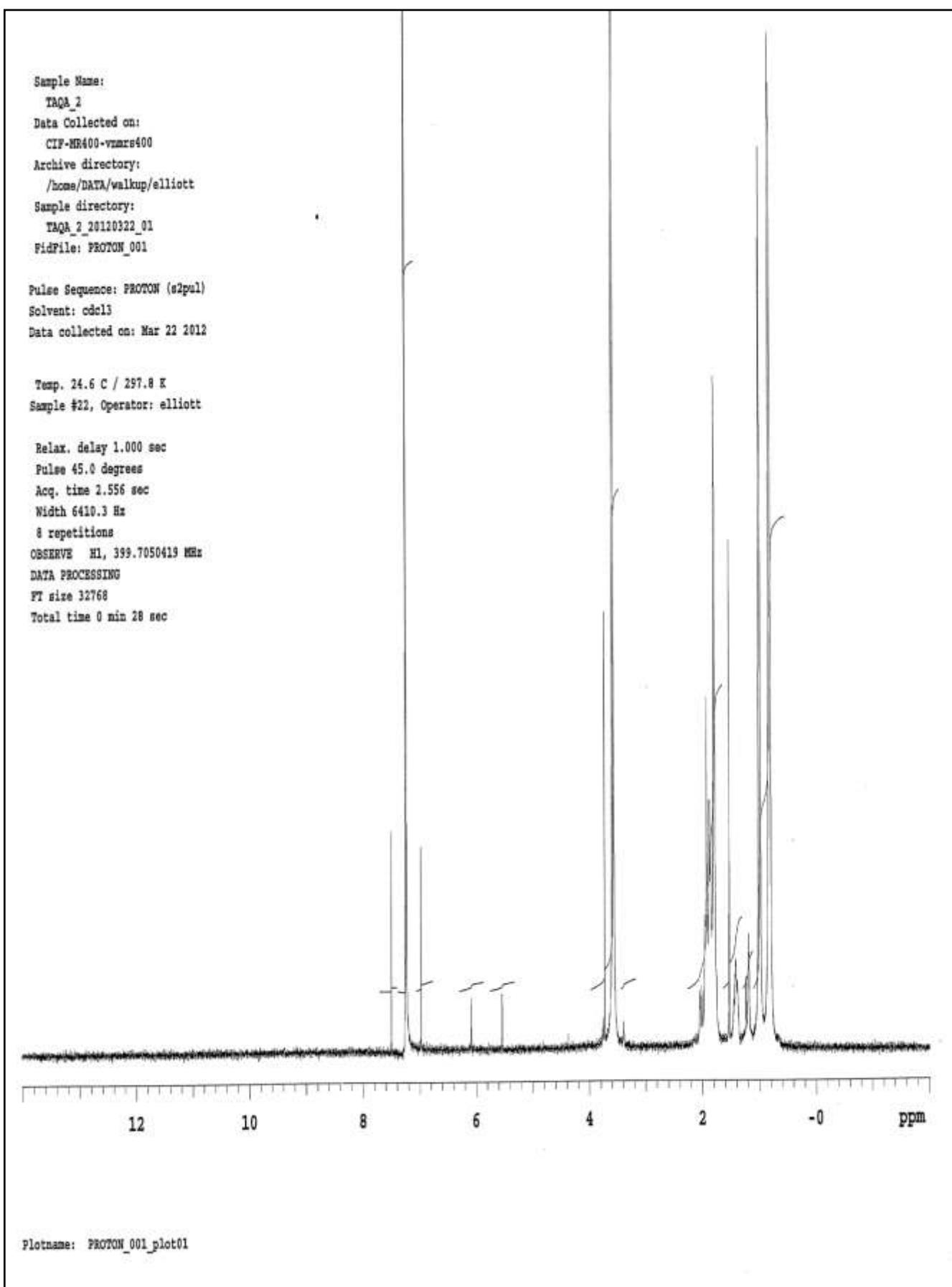


Fig (1):  $^1\text{H}$  NMR for PMMA (Pink and white acrylic) analysis

Fig.2:  $^1\text{H}$ NMR for exposed PMA (pink color)

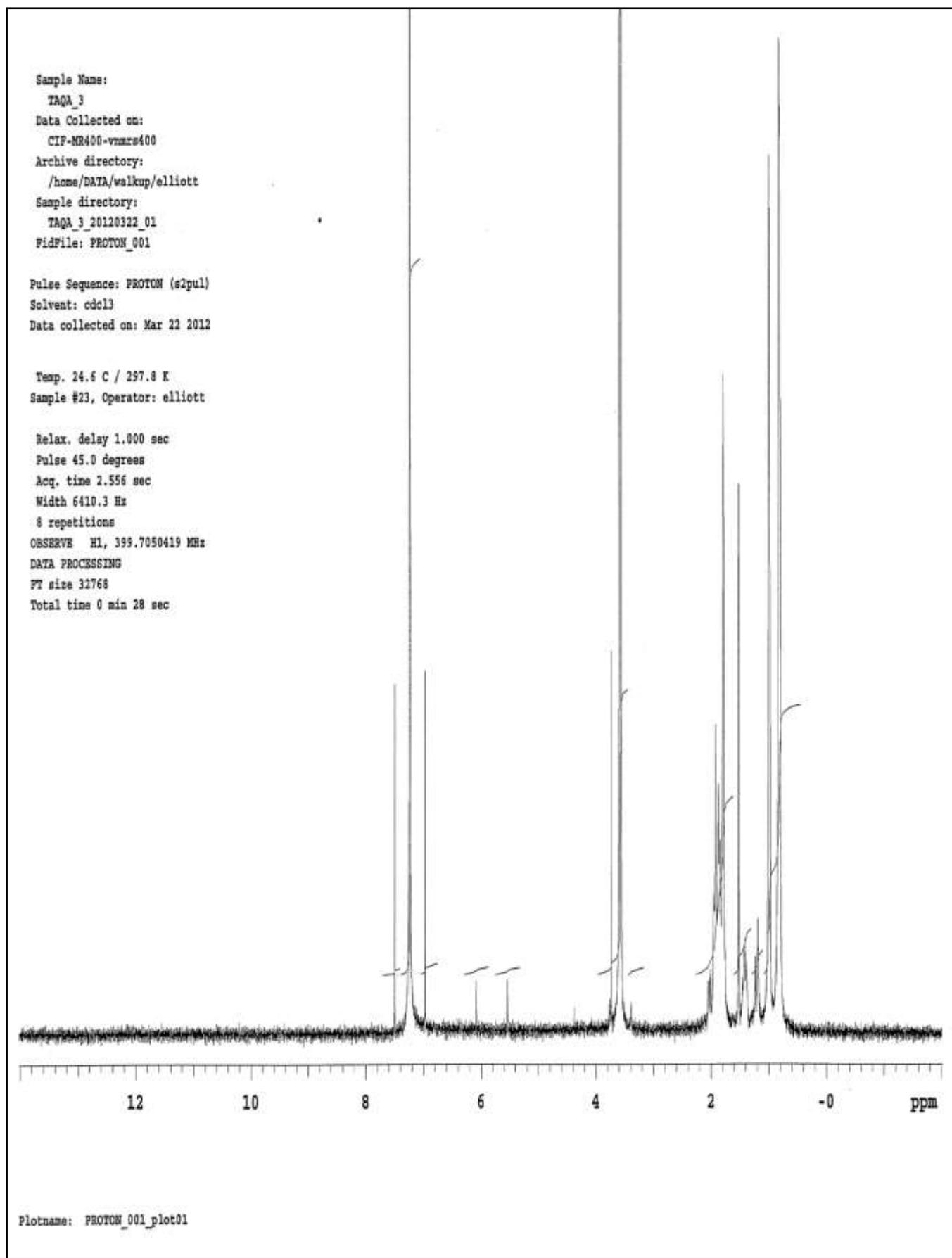
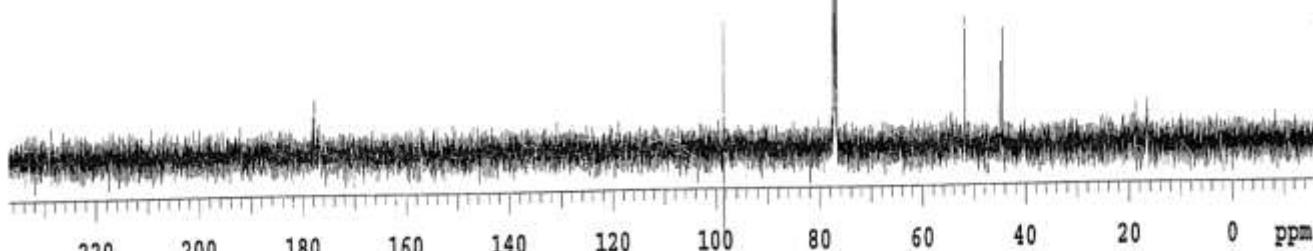


Fig.3:  $^1\text{H}$ NMR for exposed PMA (white color)

Sample Name:  
TAQA\_1  
Data Collected on:  
CIF-MR400-vnmrs400  
Archive directory:  
/home/DATA/walkup/elliott  
Sample directory:  
TAQA\_1\_20120322\_02  
FidFile: CARBON\_001  
  
Pulse Sequence: CARBON (s2pul)  
Solvent: cdcl3  
Data collected on: Mar 22 2012

Temp. 24.6 C / 297.8 K  
Sample #24, Operator: elliott

Relax. delay 1.000 sec  
Pulse 45.0 degrees  
Acq. time 1.285 sec  
Width 25510.2 Hz  
1000 repetitions  
OBSERVE C13, 100.5059127 MHz  
DECOUPLE H1, 399.7070404 MHz  
Power 38 dB  
continuously on  
WALTZ-16 modulated  
DATA PROCESSING  
Line broadening 0.5 Hz  
FT size 65536  
Total time 38 min



Plotname: CARBON\_001\_plot01

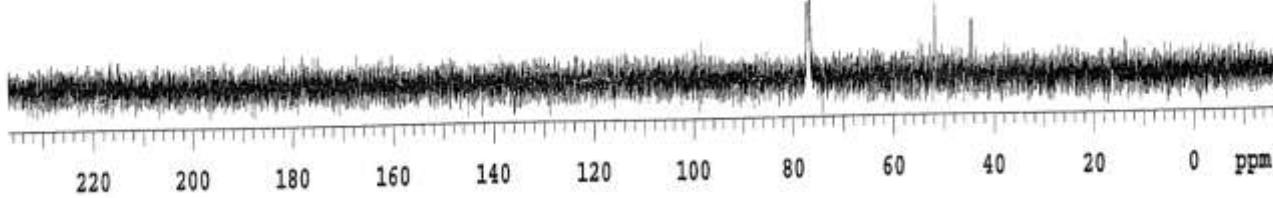
Fig (4):  $^{13}\text{C}$  NMR (Pink acrylic) powder analysis

Sample Name:  
TAQA\_3  
Data Collected on:  
CIF-MR400-vmars400  
Archive directory:  
/home/DATA/walkup/elliott  
Sample directory:  
TAQA\_3\_20120322\_01  
PifFile: CARBON\_001

Pulse Sequence: CARBON (s2pul)  
Solvent: cdcl3  
Data collected on: Mar 22 2012

Temp. 24.6 C / 297.8 K  
Sample #23, Operator: elliott

Relax. delay 1.000 sec  
Pulse 45.0 degrees  
Acq. time 1.285 sec  
Width 25510.2 Hz  
1000 repetitions  
OBSERVE C13, 100.5059127 MHz  
DECOUPLE H1, 399.7070404 MHz  
Power 18 dB  
continuously on  
WALTZ-16 modulated  
DATA PROCESSING  
Line broadening 0.5 Hz  
FT size 65536  
Total time 38 min



Plotname: CARBON\_001\_plot01

Fig (5):  $^{13}\text{C}$  NMR for PMMA (pink color)

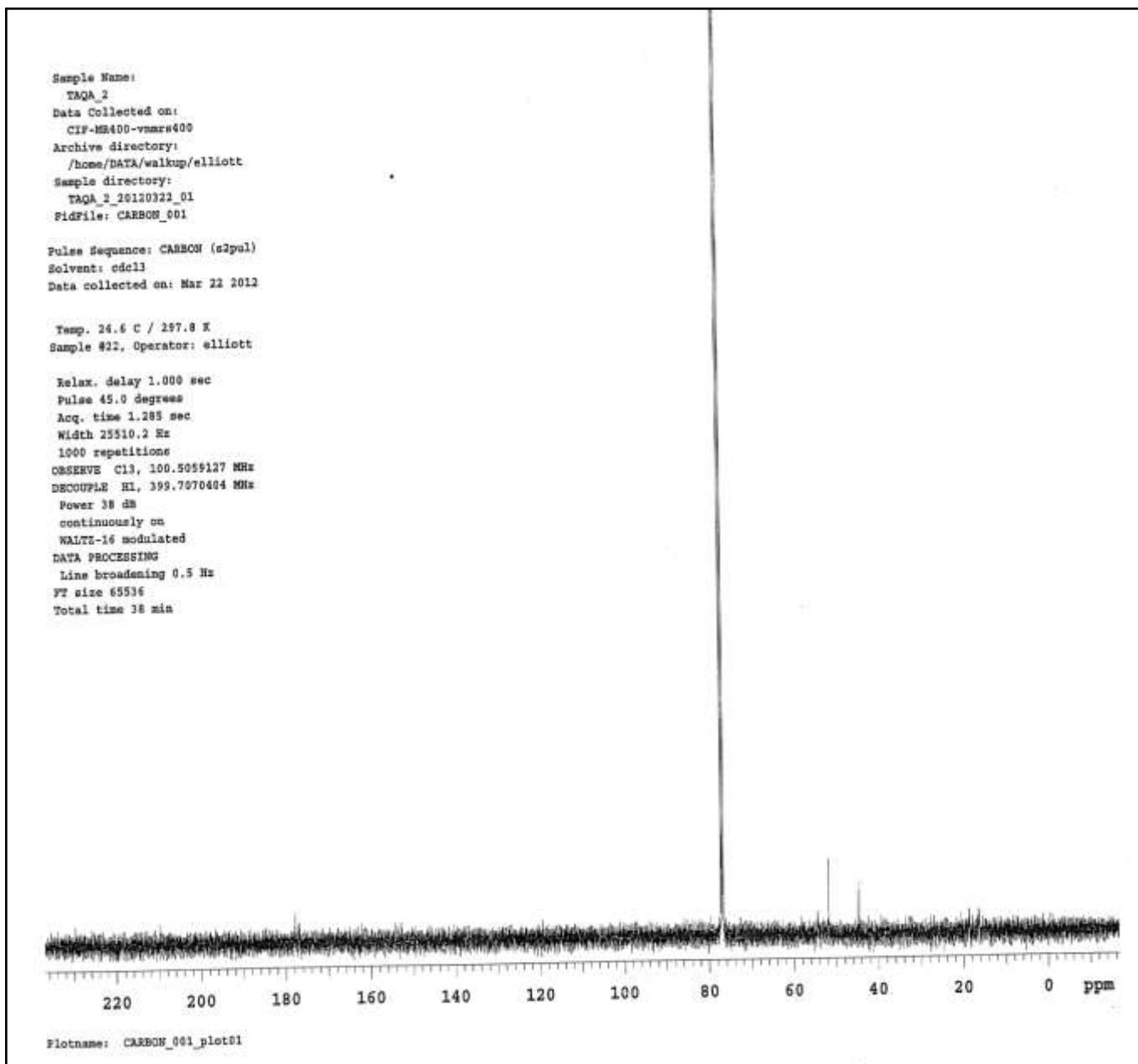


Fig (6):  $^{13}\text{C}$  NMR for PMMA (white color)

## DISCUSSION

(NMR) spectra analysis is one of most commonly and widely disappeared and promising analytic study for chemical and bio-chemical analytic study and it is become very durable test in structural build up analysis and changes evaluation with study <sup>(15)</sup>. The results obtained by this test is mainly based on chemical analysis of polymethyl methacrylate powder, and the results showed that polymethyl polymer chemically not showed any change in the chemical structure after exposure to MRI, this results was confirmed by studying  $^1\text{H}$ NMR and  $^{13}\text{C}$  NMR spectroscopy. The characters but since their main chemical structure remain unchanged, so major changes have been expected to happened in their chemical properties, although this is now under study, and further researcher, in future will expected to be promising and nearly. Restricting about weather exposure to MRI is safe or not.

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