Electronic Magnetic Resonance Spectrum of Some Organic Materials

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قال تعالى: (فَتَعَالَى اللَّهُ الْمَلِكُ الْحَقَّ وَلَا تَعْجَلْ بِالْقُرْآنِ) وَقُل رَّبَِّ زِدْنِي عِلْمًا

سورة طه الآية 114
Dedication

To my father and mother

To my family

To may all real friends

To all those who help

Maser

Degree
Acknowledgments

All praise is to Allah almighty; who are the one and only creator of this whole universe, thanks are to the University of Gezira and all professors of the department of Electronic Engineering Faculty of Engineering and Technology.

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Electronic Magnetic Resonance Spectrum of Some Organic Materials

Nagla Mohammed Abd Algani Osman

Department of Electronics Engineering

M. Sc. Physics

Abstract

Magnetic Resonance is the phenomena in which an external magnetic field applied to an atom split the energy level into sub levels. The energy difference between these sub levels is proportional to the magnetic field strength. Electron Spin Resonance is technique for studying chemical species that have one or more unpaired electrons such free radicals. Electrons having spin in the direction of the external magnetic field occupy lower sub level, while those having spin in the direction opposite to that of the external field occupy upper sub level. When a photon of appropriate energy equal to the difference between the two levels is incident on the atom, the photon is absorbed by an electron in the lower sub level and it make transition to the upper sub level. Thus resonance takes place due to this photon absorption. The aim of this study to obtain electronic resonance spectrum to use instead of nuclear magnetic resonance spectrum. This was applied to four sample ( water, methanol, hexanol and N,N – Dimethyl formamaide) , to measure wave length and chemical shift,δis (δ ,ppm) and comparing results between electronic magnetic resonance spectrum and nuclear magnetic resonance spectrum , water gives a frequency 5.34x10^{14} Hz while in the chemical shift,δis (δ , ppm) 1.24 , 1.33 , 1.56 and methanol gives frequency is 4.24 x10^{14} Hz ,4.52 x10^{14} Hz , 4.83 x10^{14} Hz while the chemical shift,δ is(δ,ppm) 3.24, 3.34 ,3.49 and hexanol frequency 4.8x10^{14} Hz , 5. 52x10^{14} Hz while the chemical shift,δis (δ,ppm) 0.76,0.81,0.88 and N,N – Dimethyl formamide frequency is 5.35x10^{14} Hz, 4.15x10^{14} Hz while in chemical shift,δis (δppm) 7.8,8.1,8.2. These results were compared with nuclear magnetic resonance spectrum and they were found very near within references. Due to these results nuclear magnetic resonance spectrum can be used as reference this agrees with the fact that these organic compounds emit the same photon within the
visible spectrum range. This study recommended that more investigations are needed to apply in other organic compounds.
طيف الرنين النووي الإلكتروني لبعض المواد العضوية

نجلاء محمد عبد الغني عثمان
قسم هندسة الإلكترونيات
ماجستير العلوم في الفيزياء
ماجستير العلوم في الفيزياء

ملخص

الرنين المغناطيسي هو الظاهرة التي يتم فيها تطبيق مجال مغناطيسي خارجي على الذرة حيث ينفق مستوى الطاقة مستويات فرعية ويكون الفرق في الطاقة بين هذه المستويات الفرعية متناسقاً طردياً مع شدة المجال المغناطيسي المطبق، والرنين المغزلي الإلكتروني طريقة لدراسة المواد التي تحتوي على إلكترونات غير متزاوجة. وتحتل الإلكترونات ذات المغزلي المضاد لاتجاه المجال المغناطيسي تحت مستوى الطاقة الأدنى بينما تلك ذات المغزلي المضاد لاتجاه المجال المغناطيسي تحت مستوى الطاقة الأعلى. وعند سقوط فوتون طاقته تساوي طاقة الفرق بين المستويين يتم امتصاص الفوتون بواسطة الإلكترون في المستوى الفرعي الأدنى ويحدث له انقلال للمستوى الفرعي الأعلى. إذاً يحدث رنين نتيجة لامتصاص هذا الفوتون. الهدف من هذه الدراسة هو الحصول على طيف الرنين الإلكتروني لاستخدامه بدلاً من طيف الرنين النووي المغناطيسي ثم تطبيقه في أربعة عينات هي (الماء، الهكسانول، الهكسانول، الهكسانول)، و N,N-ثنائي ميثيل فورمايد) لقياس التردد والإزاحة الكيميائية ومقارنة نتائج طيف الرنين النووي المغناطيسي وطيف الرنين النووي الإلكتروني وطيف الرنين النووي المغناطيسي وجد أن الماء يعطي تردد 5.34x10^14 Hz بينما الإزاحة الكيميائية 1.69, 1.33, 1.24 والهكسانول تردد 4.83x10^14 Hz - 4.24x10^14 Hz - 4.52x10^14 Hz - 5.52x10^14 Hz بينما الإزاحة الكيميائية 4.8x10^14 Hz-5.52x10^14 Hz-3.49, 3.24 والهكسانول يعطي تردد 4.15x10^14 Hz بينما الإزاحة الكيميائية 0.76, 0.81, 0.88 ثنائي ميثيل فورمايد بينما الإزاحة الكيميائية 5.35x10^14 Hz, بينما الإزاحة الكيميائية 8.2, 8.1, 7.8. وقورنت هذه النتائج مع نتائج الرنين النووي المغناطيسي وكانت النتائج مقاربة معها. كما في المراجع. توصي هذه الدراسة بمزيد من الاختبارات للنظر في كيف تبدو أطيف الرنين المغناطيسي لمركبات عضوية أخرى.
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Chapter One

Introduction

1.1 Overview

The discovery of magnetic field dates from the early Greek, discovery that certain stones, called magnetite, attract iron pieces, the car pass which was magnetic head is attracted by their stone (Kittle, c.1976).

The magnetic field is utilized in a wide variety of application. It can be used to produce electricity by electric generates, beside its application in petroleum exploration, the magnetic field is now a day utilized in curing some diseases, which is now represents the basis of anew breach of medicine known as magneto therapy (Tsui, Dc. Stormer and others 1982) It is also used as probe for diagnosis (A.), where the so called magnetic resonance imaging (MRI) (Khwjali, A 2009)

Is now considered as one of the most power full accurate diagnosing tool in diagnosis of soft tissues.

The study of atomic structure by scientists using quantum law shows that electrons, nuclei, and atoms can act as small tiny magnets. The electrons are located in certain orbits around the nucleus. Applying magnetic field lead to spotting of each orbit to sub levels. When a photon of appropriate frequency is applied, electrons absorb this photon to make transition between these subsorbit this phenomena is known as magnetic resonance (Halliday and others 1974).

1.2 Research Problem

The research problem is related to the fact that most of the medical researchers are related to nuclear spin resonance; no intensive research is made for electron spin resonance.
1.3 The Aim of the Work

The aim of this work is to study the properties of some organic components in the form of fluid by using electron spin resonance technique.

1.4 layout of Thesis

The thesis consists of Five Chapters, Chapter one Introduction, Chapter Two Theatrical Background, Chapter Three Magnetic Resonance and Chapter Four the Result Chapter Five Discussion and Recommendation.
Chapter Two
Theoretical Background

2.1 Introduction

This chapter is concerned with the magnetic properties of matter. This includes magnetic susceptibility, super conductors, cooper pairs, energy gap in superconductors, London equation’s, derivation of first London equation, second London equation, London penetration depth in superconductors, magnetic flex quantization of superconductor lengvein equation Zeeman effect, and quantum half effect (A. Khagali 2000).

2.2 Magnetic Moment and susceptibility

The magnetic moment $P_0$ is defined, in terms of the current $i$ and the area $A$ enclosed by it, to be in the form (Bashie.M2004).

$$P_0 = iA \quad (2.2.1)$$

But the current generated by the electron of charge moving around a nucleus in a circular orbit of radius is given by:

$$i = -ef = \frac{e\omega}{2\pi} \quad (2.2.2)$$

$f \equiv frequency$

Where the area is given by:

$$A = \pi r^2 \quad (2.2.3)$$

On the other hand the orbital angular $L$ is given by (2.2.5):

$$L = mvr = m\omega r^2 \quad (2.2.4)$$
Where \( m \) is the mass electron and \( V \) is the electron speed.

Inserting (2.2.2), (2.2.3) and (2.2.4) in (2.2.1) yields the magnetic moment in the form:

\[
P_0 = iA = -\frac{e\omega}{2\pi}(\pi r^2) = -\frac{e\omega r^2}{2}
\]

\[
P_0 = \frac{-em\omega r^2}{2m} = \frac{-e}{2m} \vec{L}
\]  (2.2.5)

Similarly the spin magnetic moment \( P_s \) is related to the spin angular momentum according to the relation:

\[
\vec{P}_s = \frac{-e}{m} \vec{S}
\]  (2.2.6)

The total magnetic moment \( P_m \) resulting from spin and orbital motion is given by (2.2.5)

\[
\vec{P}_m = \frac{e\hbar}{2m} g_J \vec{J}
\]

\[
\vec{P}_m = -\mu g_i \vec{J}
\]  (2.2.7)

\( \vec{J} \) is the quantum number, \( g_J \) is the \( g \) factor and \( \mu_g \) is the susceptibility. Hence

\[
\vec{P}_m = \mu_B(\vec{L} + 2\vec{S})
\]  (2.2.8)

Where

\[
g_J \vec{J} = (\vec{L} + 2\vec{S})
\]  (2.2.9)

\[
\mu_B = \frac{e\hbar}{2m}
\]  (2.2.10)
The parameter $g_J$ can simply be given by

$$g_J = \frac{3/2 \hat{j}^2 + \left(\frac{1}{2}\right) \hat{S}^2 - \frac{1}{2} \hat{L}^2}{\hat{j}^2} = \frac{3}{2} + \frac{S(S + 1) - L(L + 1)}{2J(J + 1)}$$

(2.2.11)

$$\hat{j} = \hbar \sqrt{J(J + 1)}$$

(2.2.12)

This relation can be found by setting

$$\hat{j} = \mathbf{L} + \hat{S}$$

(2.2.13)

$$J^2 + L^2 + S^2 + 2\mathbf{L} \cdot \hat{S}$$

(2.2.14)

$$(\mathbf{L} + 2\hat{S}) = \mathbf{L} + 2\hat{S}$$

(2.2.15)

To

$$g_J \hat{j} \cdot \hat{j} = (\mathbf{L} + 2\hat{S}) \cdot (\mathbf{L} + \hat{S}) = L^2 + 2S^2 + 3\mathbf{L} \cdot \hat{S}$$

(2.2.16)

Then

$$g_J J^2 = L^2 + 2S^2 + 3L \cdot S$$

(2.2.17)

From (2.2.14)

$$L \cdot S = \frac{J^2 - L^2 - S^2}{2}$$

$$= \frac{1}{2} J^2 - \frac{1}{2} L^2 - \frac{1}{2} S^2$$

$$g_J J^2 = L^2 + 2S^2 + \frac{3}{2} J^2 + \frac{3}{2} L^2 - \frac{3}{2} S^2$$

$$= \frac{3}{2} J^2 - \frac{1}{2} L^2 + \frac{1}{2} S^2$$
Hence

\[ g_J = \frac{3}{2}f^2 - \frac{1}{2}S^2 - \frac{1}{2}L^2 \]  

(2.2.18)

If \( n \) atoms per unit volume align themselves along the x-axis thus the component is given by

\[ M_x = nP_m = -n\mu_B g_J \hat{J} \]  

(2.2.19)

Where \( M_x \) changes from \( 0 \) to \( \max \) value during a time \( T \).

The electron revolving around a nucleus can produce a magnetic field of flux density \( B \). If the electron revolves with frequency \( f \) in circular orbit of radius \( r \), then according to Bio-savart law it produces a magnetic field of flux density (Charles K, 2004)

\[ B_e = \frac{\mu_0 i}{2r} \]  

(2.2.20)

\[ B_e = \frac{\mu_0 fe}{2r} \]  

(2.2.21)

Hence

\[ i = fe \]

The magnetic moment produced by such an electron is given by

\[ P_m = iA = i(\pi r^2) = \pi ir^2 \]  

(2.2.22)
For \( Z \) electrons with mean radius \( r \), the magnetic flux density of the atom \( (B_a) \) is given by

\[
B_a = \frac{\mu_0 Z f e}{2r} \tag{2.2.23}
\]

Thus the internal atomic field generated by one electron \( B_i = \frac{\mu_0 f e}{2r} \) and is related to the magnetic moment through the relation

\[
B_e = \frac{\mu_0 P_m}{2\pi r^3} \tag{2.2.24}
\]

Since the current for the whole atom is

\[
i = Z f e
\]

Hence the field of the atoms is related to the magnetic moment also as follows:

\[
B_a = \frac{\mu_0 P_m}{2\pi r^3} \tag{2.2.25}
\]

But the magnetic moment \( M \) is defined in terms of the number of dipoles \( N \) divided by the volume \( V \) to be

\[
M = \frac{N P_m}{V} \tag{2.2.26}
\]

If the atomic radius is \( r' \), thus one atom exists in a volume \( V_a \) is given by

\[
\frac{N}{V} = \frac{1}{V_a} = \frac{1}{\frac{4}{3}\pi r'^3} = \frac{3}{4\pi r^3} \tag{2.2.27}
\]

This

\[
M = \frac{3 P_m}{4\pi r^3} \tag{2.2.28}
\]
Using (2.2.24), (2.2.27) and (2.2.28) in (2.2.29) yields

\[ M = \frac{3}{4\pi r^3} \frac{B_a}{\mu_0} (2\pi r^3) = \frac{3B_a}{2\mu_0} \]  

(2.2.29)

2.3 Magnetic Materials Types

The magnetic materials are either diamagnetic or paramagnetic or ferromagnetic:

1-In diamagnetic materials an atom have on magnetic moment and does not act as a tiny small magnet, where they have even number of electrons. When an external magnetic field is applied, atomic electrons induce current that generates a magnetic field that opposes the applied external magnetic field and tend to cancel it inside the diamagnetic material. Thus diamagnetic material tends to decrease the external magnetic field. When the external field is turned off the induced magnetic field vanishes.

2-Paramagnetic materials atoms act as a small tiny magnet when an external magnetic field is applied the atomic magnetic tend to align themselves in the direction of the applied magnetic field. Thus it increases the magnetic fluxes density inside the paramagnetic material (David, and other 2006).

But when the external magnetic field is removed atomic magnetic return back to their random state due to the effect of random thermal motion. Atoms have odd number of electrons.

3-In ferromagnetic material atoms, have even number of electrons, and acts as small magnet. When an external magnetic field is applied atomic magnets align themselves in the direction of the field.

However, the atoms which are heavy and accumulated in domains, does not returns to their random original state.

Thus the ferromagnetic material acts as. Permanent magnet.
2.4 Lang vein Diamagnetic

If one have an electron an atom, forces act on it one is the electric force $F_e$ and the other is the centrifugal force $F_c$. Thus the equation of motion is given by Einstein (A.plancks.1907).

$$\frac{mv^2}{r} = m\omega^2 r_0 = F_c = F_y$$

(2.4.1)

Where

$m \equiv mass$

$v \equiv \omega r \equiv velocity$

$r_0 \equiv radius$

$\omega_0 \equiv angulae velocity$

When the electron is to magnetic field of flux density $\beta$, the equation of motion be care

$$\frac{mv^2}{r_0} = m\omega^2 r_0 = F_g + Bev = F_g + Be\omega r_0$$

(2.4.2)

Thus

$$m\omega^2 r_0 = m\omega_0^2 r_0 + Be \omega r_0$$

Therefore

$$m(\omega^2 - \omega_0^2) = Be\omega$$

If one assumes that the original and new frequency are nearly equal

$$\omega - \omega_0 = \Delta\omega = \omega_L$$
Where
\[ \omega \approx \omega_0 \]  

(2.4.3)

Hence

\[ m(\omega - \omega_0)(\omega + \omega_0) = Be\omega \]

\[ m(\omega_L)(2\omega) = Be\omega \]

Thus the Lamer angular frequency became

\[ \omega_L = \frac{Be}{2m} \]  

(2.4.4)

In this case a current is generated, with

\[ i = -Ze\omega_L = -Ze\frac{\omega_L}{2\pi} \]

\[ i = \frac{-Ze^2\beta}{4\pi m} \]  

(2.4.5)

In this case the atomic magnetic moment becomes

\[ M_a = iA \quad A = \pi r_0^2 \]

\[ M_a \equiv \text{atom} \]

\[ A \equiv \text{orbitarea} \]

Thus:

\[ M_a = \frac{-Ze^2\beta(\pi r_0^2)}{4\pi m} \]

\[ M_a = \frac{-Ze^2\beta}{4m} \frac{r_0^2}{r_0^2} \]  

(2.4.6)
As a result the magnetic moment per unit volume became

\[ M = nM_a = \frac{-Ze^2 \beta n}{4m} r_0^2 \]  

\[ n \equiv \text{density of atom} \]

Fig (2.4.1) radius Lang evin Diamagnetic

\[ r^2 = x^2 + y^2 + z^2 \]

If

\[ z = x = y \]

\[ :. r^2 = 3z^2 \]

\[ z^2 = \frac{1}{3} r^2 \]

But

\[ R^2 + Z^2 = r^2 \]

\[ r_0^2 = R^2 = r^2 - Z^2 = r^2 - \frac{1}{3} r^2 = \frac{2}{3} r^2 \]  

(2.4.8)
It follows that

\[ M = \frac{-2Ze^2r^2n\beta}{3 \times 4m} \]

\[ = \frac{-Ze^2nr^2\mu_0}{6m}H \]

\[ = \chi H \quad (2.4.9) \]

Where \( \chi \) is the magnetic susceptibility's Thus the diamagnetic susceptibility

\[ \chi = \frac{-nZe^2n\mu_0r^2}{6m} \quad (2.4.10) \]

### 2.5 Quantum Paramagnetic Materials

Consider a magnetic field of strength \( H \) is applied a Para-magnetic materials. In this case electrons having positive spin align themselves in direction opposite to the applied external field, and their energy increase. In contrary those of negative spin align themselves in the direction of the external field and their energy decreases (R.AbdElhaietal 2013).

\[ \Delta E = g\beta Hm_s \quad (2.5.1) \]

Fig (2.5.1) The energy change due to the application of magnetic field.
Where

\[ g \equiv \text{landan factor} \]

\[ \beta \equiv \text{Boher magneton} \]

\[ m_s \equiv \text{magnetic spin quantum number} \]

\[ H \equiv \text{magent} \]

Consider now the total number of particles in state \( E_1 \) and \( E_2 \) is given by

\[ n = n_1 + n_2 \]

The number of particles in state \( E_1 \) and \( E_2 \) can be described by Maxwell distribution where

\[ n_1 = e^{\frac{\Delta E}{kT}} = e^x; \quad n_2 = e^{-\frac{\Delta E}{kT}} = e^{-x} \]

The \( x \) is defined by

\[ x = \frac{\Delta E}{kT} \quad (2.5.2) \]

The magnetic moment \( M \) is the moment due to spin up and spin down atomic moments, therefore

\[ M = g\beta m_s(n_1 + n_2) \quad (2.5.3) \]
Hence

\[ M = g\beta m_s \frac{(e^x - e^{-x})}{n} n = g m_s \beta \frac{(e^x - e^{-x})}{(e^x + e^{-x})} n \]

\[ = \frac{(1 + x - 1 + x)}{1 + x + 1 - x} g m_s \beta n \]

\[ g m_s \beta n \chi = \frac{ng^2 m_s^2 \beta^2 H}{kT} \]  \hspace{1cm} (2.5.4)

If one substitute

\[ = g = 2 \quad m_s = \frac{1}{2} \]

The paramagnetic susceptibility is given by

\[ \chi = \frac{M}{H} = \frac{n\beta^2}{kT} \]  \hspace{1cm} (2.5.5)

2.6 Magnetic Resonance:

First observation of an electron spin resonance (e.s.r) spectrum was reported by a Russian, E. Zaviosky. In 1945 conceptually, the scientific climate had probably been right for the experiment some ten years earlier, for a Dutch school of physicist, led by c.j Garter was concerned with the adiabatic demagnetization method of achieving very low temperatures Technologically, however. The experiments only become reasonably feasible after the Second World War had catalyses the development of microwave techniques (Hugo, 1997).

2.7 Electron and photon spin Magnetic Moment

Magnetic field is generated by moving charges, when a charge moves around itself or around a certain point, magnetic field is generated.

Consider now an electron of charge moves in circus orbit density \( B \) generated is given by (Servey, and other 2004):
\[ B_e = \frac{M_e i}{2r} = \frac{\mu_0 f_e}{2r} \]  

(2.7.1)

Where

\[ \mu_0 \equiv \text{Magnetic permeability of vacuum} \]

\[ i \equiv \text{electric current} \]

\[ f \equiv \text{electron frequency} \]

(Number of revolution around the orbit per second).

The magnetic moment produced by this electron is given by

\[ P_m i A = i(\pi r^2) = \pi r^2 i = \mu_m = \mu \]  

(2.7.2)

\[ P_m \equiv \text{magnetic moment} \]

\[ A \equiv \text{orbit area} \]

For \( Z \) electrons the atomic magnetic field generated is given by

\[ B_a = \frac{\mu_0 Z f_e}{2r} \]  

(2.7.3)
The magnetic flux density $B_e$ and the electron magnetic moment are related according to equations and by

$$B_e = \frac{\mu_0 P_m}{2\pi r^3} \quad (2.7.4)$$

The some relation holds for atoms

$$B_a = \frac{\mu_0 P_m}{2\pi r^3} \quad (2.7.5)$$

The magnetic moment of the whole body or material is the average magnetic moment per unit volume. Thus if the a number of atoms per unit volume is $n$. Thus the magnetic moment is given by

$$M = nP_m \quad (2.7.6)$$

The magnetic moment is related to the orbital angular momentum $L$ is given by

$$L = mvr = m(\omega r)r = m(2\pi f) r$$

$$= m(2\pi f)r^2$$

$$= \frac{m}{e}(-ef)(\pi r^2) = \frac{-2m}{e} iA = \frac{-2m}{e} \mu_m$$

Thus

$$M_m = -\left(\frac{e}{2m}\right)L \quad (2.7.7)$$

The some relation holds for spin angular momentum

$$M_s = -\left(\frac{e}{2m}\right)S \quad (2.7.8)$$
Where

\( M_s \equiv \text{spin magnetic momentum} \)

\( S \equiv \text{spin angular momentum} \)

### 2.8 Zeeman Effect

Zeeman Effect is the effects that study the interaction between magnetic moment of atoms or electrons or protons with the external magnetic field.

This interaction can be described by the potential energy gained due to the force excreted the potential energy gained is given by (R.AbdElhai etal., 2013).

\[
V_m = \int F ds = \int Fr d\theta = \int qBr d\theta = \int (qr)B d\theta = \int M.B d\theta = \int MBcos\phi d\theta = \int MBsin\theta d\theta
\]

\[MBcos\phi = \mu_mBcos\theta\] (2.8.1)

![Fig: (2.8.1) The Tragus on the magnetic moment](image)

Where:

\( F = qB \equiv \text{force} \)

\( q \equiv \text{magnetic charge} \)
\[ qr = \mu \equiv \text{magnetic moment} \]

The magnetic torque is given by:

\[ \tau = \mu B \sin \theta \quad (2.8.2) \]

The magnetic potential generated by the electron or proton is given by using equations (2.7.7) and (2.8.1) to be

\[ V_m = -\mu_m B \cos \theta = \left( \frac{e}{2m} \right) L B \cos \theta \quad (2.8.3) \]

The \( Z \) component of \( L \) is given by

\[ L \cos \theta = L_Z \]

Thus equation (3.3.3) redoes to

\[ V_m = \left( \frac{e}{2m} \right) L_Z \quad (2.8.4) \]

Since electrons and protons quantum L end, thus one replace \( L_Z \) by the magnetic orbital quantum number \( m_L \) to get

\[ V_m = \left( \frac{e}{2m} \right) B m_L \quad (2.8.5) \]

Where the volumes of \( m_L \) are

\[ m_L = \pm 1 \]

However when the magnetic field effect spin magnetic moment one do the following replay

\[ L \rightarrow S \quad L_Z = S_Z \quad (2.8.6) \]

\[ m_L \rightarrow m_S \]
To get

\[ V_m = \left( \frac{e}{2m} \right) B_S \cos \theta = \left( \frac{e}{2m} \right) B_{SZ} \quad (2.8.7) \]

\[ V_m = \left( \frac{e}{2m} \right) B_{mS} \quad (2.8.8) \]
Chapter Three

Material and Methods

3.1 Introduction

Nuclei with an odd mass or odd atomic number have "nuclear spin" (in a similar fashion to the spin of electrons). This includes $^1$H and $^{13}$C (but not $^{12}$C). The spins of nuclei are sufficiently different that NMR experiments can be sensitive for only one particular isotope of one particular element. The NMR behavior of $^1$H and $^{13}$C nuclei has been exploited by organic chemist since they provide valuable information that can be used to deduce the structure of organic compounds. These will be the focus of our attention. Since a nucleus is a charged particle in motion, it will develop a magnetic field. $^1$H and $^{13}$C have nuclear spins of $\frac{1}{2}$ and so they behave in a similar fashion to a simple, tiny bar magnet. In the absence of a magnetic field, these are randomly oriented but when a field is applied they line up parallel to the applied field, either spin aligned or spin opposed. (Ashcroft , and other 1976 ) The more highly populated state is the lower energy spin state spin aligned situation. Two schematic representations of these arrangements are shown in fig (3.1.1).

![Fig (3.1.1) NMR two schematic representations spin situation](image-url)
In NMR, electromagnetic (EM) radiation is used to "flip" the alignment of nuclear spins from the low energy, spin aligned state to the higher energy spin opposed state. The energy required for this transition depends on the strength of the applied magnetic field (see below). The energy difference between the spin states is quite small and corresponds to the radio frequency range of the EM spectrum (Francis Fiche, 2013).
As this diagram shows, the energy required to cause the spin-flip, $\Delta E$, depends on the magnetic field strength at the nucleus. With no applied field, there is no energy difference between the spin states, but as the field increases, so does the separation of energies of the spin states and therefore so does the frequency required to cause the spin-flip.

$\Delta E' > \Delta E$ since $H_o' > H_o$

**Fig (3.1.4) Increasing magnetic field**

**Fig(3.1.5) The basic arrangement NMR spectrometer**
3.2 Chemical Shift

- An NMR spectrum is a plot of the radio frequency applied against absorption.
- A signal in the spectrum is referred to as a resonance.
- The frequency of a signal is known as its chemical shift, $\delta$

The chemical shift in absolute terms is defined by the frequency of the resonance expressed with reference to a standard compound which is defined to be at 0 ppm. The scale is made more manageable by expressing it in parts per million (ppm) and is independent of the spectrometer frequency.

$$\text{Chemical shift, } \delta = \frac{\text{frequency of signal} - \text{frequency of reference}}{\text{spectrometer frequency}} \times 10^6$$

It is often convenient to describe the relative positions of the resonances in an NMR spectrum. For example, a peak at a chemical shift, $\delta$, of 10 ppm is said to be downfield or deshielded with respect to a peak at 5 ppm, or if you prefer, the peak at 5 ppm is upfield or shielded with respect to the peak at 10 ppm. The terms shielded and deshielded will be explained (Tsui, and other 1982).

3.3 Material

- **Water**

  Water (chemical formula $\text{H}_2\text{O}$):

  Is transparent fluid which forms the world’s streams, lakes, oceans and rain, and is the major constituent fluids of organisms?

  “As a chemical compound, a water molecule contains one oxygen and two hydrogen” that is connected by covalent bonds.
• **Methanol**

  General Properties Methanol is colorless hygroscopic liquid usually containing 0.01 - 0.04 percent water. It is highly flammable and toxic. Physical Properties Molecular weight: 32.04 Freezing point (°C): -97.7 Boiling point (°C): 64.7 Flash point (°C): 11 Min. ignition temp. (°C): 455 Density (g/cm³): (0.796115 - 791320 - 0.786625) Refractive Index: (1.328420-1.326525) Viscosity (cPoise) (0.550625 0.544535) Dielectric constant: 32.7 Ionization potential (eV): 10.84 Solubility: water, organic solvents.

• **Hexanol**

  General Properties Hexanol is a colorless, water-insoluble, and highly flammable liquid. Physical Properties Molecular weight: 86.18 Freezing point (°C): -95.4 Boiling point (°C): 68.74 Flash point (°C): -26 - Min. ignition temp. (°C): 240 - Density (g/cm3): (0.659420 - 0.654825) Refractive Index: ( 0.374920 - 1.372325) Viscosity (cPoise): (0.312620 -0.298525) Dielectric constant: 1.8799 Ionization potential (eV): 10.18 Solubility: 0.00095 % in water, no polar organic solvents.

• **N,N- Dimethylformamide**

  General Properties Colorless liquid which may be obtained as the water zyotope containing about 5 percent water or as absolute alcohol containing 0.1 percent or less water. Physical Properties Molecular weight: 46.07 - Freezing point (°C): -114.1 - Boiling point (°C): 78.3 - Flash point (°C): 12 - Min. ignition temp. (°C): 425 - Density (g/cm³): 0.793615 0 -789420 0 - 78525 Refractive Index: 1.361420 1.359425 - Viscosity (cPoise): 1.07825 - 0.99135 - Dielectric constant: 24.55 - Ionization potential (eV): 10.49 Solubility: water, organic solvents
Fig(3.3.1) the experimental setup
Chapter Four
The Results

4.1 Introduction

The experimental details of this work as shown the following steps from the measurements: NMR samples (water, methanol, hexanol, and dimethyl formamide) then outcomes were.

4.2 Results

Figure (4.2.1) Relationship between Frequency and Intensity

Figure (4.2.2) Relationship between $\delta$ (PPm) and intensity
Fig (4.2.3) Relationship between Frequency ($\text{H}_z$) and Absorption (au)

**Table (4-2-1): $^1$HNMR Results of Water**

<table>
<thead>
<tr>
<th>Group</th>
<th>Frequency ($\text{H}_z$)$ \times 10^{14}$</th>
<th>Experimental $\delta$ (ppm)</th>
<th>Reference $\delta$ (ppm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Water</td>
<td>5.34</td>
<td>1.24</td>
<td>1.56</td>
</tr>
<tr>
<td></td>
<td></td>
<td>1.33</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>1.56</td>
<td></td>
</tr>
</tbody>
</table>

Experimentally determined chemical shift and that found by some researchers.
Fig (4.2.4) Relationship between frequency and intensity

Fig (4.2.5) Relationship between δ (PPm) and intensity
Table (4.2-2): $^1$H NMR Results of Methanol:

<table>
<thead>
<tr>
<th>Group</th>
<th>Frequency (Hz) x 10$^{14}$</th>
<th>Experimental $\delta$ (ppm)</th>
<th>Reference $\delta$ (ppm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Methanol</td>
<td>4.24</td>
<td>3.24</td>
<td></td>
</tr>
<tr>
<td></td>
<td>4.52</td>
<td>3.34</td>
<td>3.49</td>
</tr>
<tr>
<td></td>
<td>4.83</td>
<td>3.49</td>
<td></td>
</tr>
</tbody>
</table>

Experimentally determined chemical shift and that found by some researchers.
Fig (4.2.7) Relationship between frequency and intensity

Fig (4.2.8) Relationship between $\delta$ (PPm) and intensity
Table (4.2.9): $^1$H NMR Results of Hexanol:

<table>
<thead>
<tr>
<th>Group</th>
<th>Frequency $(\text{Hz}) \times 10^{14}$</th>
<th>Experimental $\delta$ (ppm)</th>
<th>Reference $\delta$ (ppm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Hexanol</td>
<td>4.80</td>
<td>0.76</td>
<td>0.88</td>
</tr>
<tr>
<td></td>
<td>5.52</td>
<td>0.81</td>
<td></td>
</tr>
</tbody>
</table>

Experimentally determined chemical shift and that found by some researchers.
Fig (4.2.11) Relationship between δ (ppm) and intensity

Fig (4.2.10) Relationship between frequency and intensity
Fig (4.2.12) Relationship between Frequency (Hz) and Absorption (au)

Table (4 -2 -4): $^1$H NMR Results of N,N – Dimethyl Formamide :

<table>
<thead>
<tr>
<th>Group</th>
<th>Frequency (Hz) x 10$^{14}$</th>
<th>Experimental $\delta$ (ppm)</th>
<th>Reference $\delta$ (ppm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Dimethyl</td>
<td>4.15</td>
<td>7.8</td>
<td></td>
</tr>
<tr>
<td></td>
<td>5.35</td>
<td>8.1</td>
<td>8.2</td>
</tr>
</tbody>
</table>

Experimentally determined chemical shift and that found by some researchers.
Table (4.2.5) $^1$H NMR Data

<table>
<thead>
<tr>
<th>Group</th>
<th>CD Cl₃</th>
<th>(CD₃)$_2$ CO</th>
<th>(CD₃)$_2$ SO</th>
<th>D₂ O</th>
</tr>
</thead>
<tbody>
<tr>
<td>Water</td>
<td>1.56</td>
<td>2.84</td>
<td>3.33</td>
<td>-</td>
</tr>
<tr>
<td>Methanol</td>
<td>3.49</td>
<td>3.31</td>
<td>3.16</td>
<td>3.34</td>
</tr>
<tr>
<td>Hexanol</td>
<td>0.88</td>
<td>0.88</td>
<td>0.86</td>
<td>-</td>
</tr>
<tr>
<td>Dimethyl formamide</td>
<td>8.02</td>
<td>7.96</td>
<td>7.95</td>
<td>7.92</td>
</tr>
</tbody>
</table>

*Source (Hugo E. et al., 1997)*
Chapter Five

Discussion and Recommendation

5.1 Discussion

The analysis of the spectrum of (water, methanol, hexanol and N,N-Dimethyl formamaide) shows that the intensity beaks lie within the range of visible spectrum. Where the range of peaks is $3 - 5 \times 10^{14} \text{Hz}$. This range corresponds to wave length range $100 - 500 \text{nm}$. This range includes visible light range. This means that transition of electrons between energy levels of the atoms or molecules of the compounds results in emission of photons in the visible and near the visible range. This agree with the fact that the $H$ atoms and $O$ atoms emit photons within the ranges obtained by using magnetic resonance technique. It is very interesting to note that the chemical shift obtained for these compounds are in the permissible range, and are affected by chemical structure the presence of impurities. The effect of chemical structure and impurities can be clearly observed in the work of (Hugo) where the chemical shift ranges from 0.04 up to 4.37 due to the changes of water chemical structure and impurities.

5.2 Conclusion

In the work study to obtain electronic resonance spectrum to used instead of nuclear magnetic resonance spectrum the organic material were select like (water, methanol, Hexthanol and N,N – Dimethyl formamaide), and measured wave length and chemical shift, $\delta$ (\(\delta\), ppm) and comparing results between electronic magnetic resonance spectrum and nuclear magnetic resonance spectrum, water a frequency $5.34 \times 10^{14} \text{Hz}$ while in the chemical shift, $\delta$ (\(\delta\), ppm) 1.24, 1.33, 1.56 and methanol a frequency $4.24 \times 10^{14} \text{Hz}$, $4.52 \times 10^{14} \text{Hz}$ and $4.83 \times 10^{14} \text{Hz}$ while the chemical shift, $\delta$ is (\(\delta\), ppm) 3.24, 3.34, 3.49 and hexthanol frequency $4.8 \times 10^{14} \text{Hz}$, $5.52 \times 10^{14} \text{Hz}$ while the chemical shift, $\delta$ is (\(\delta\), ppm) 0.76, 0.81 and 0.88 and N,N – Dimethyl formamide frequency is $5.35 \times 10^{14} \text{Hz}$, $4.15 \times 10^{14} \text{Hz}$ while in chemical shift, $\delta$ is (\(\delta\), ppm) 7.8, 8.1 and 8.2. The results were compared with nuclear magnetic resonance spectrum and they
were found the results very near within references. Also can be used the electronic resonance spectrum analysis some Organic material with in nuclear magnetic resonance.

3.5 Recommendation

This study recommended that more investigation needed to apply in other organic compounds.
4.6 References:


   Doi.10.1103/phyRevLett.48.1559.


L. R.AbdElhaietal " using tight binding approximation in deriving the quantum critical temperature super conductivity equation natural , V.5, N.8 , 941-946(2013).


