

**REVIEW OF NMR SPECTROSCOPY: BASIC PRINCIPLES,  
CONCEPTS AND APPLICATIONS IN MEDICAL AND DENTISTRY****Khushnuma F. Elavia\* and Parinaz F. Elavia**Article Received on  
07 May 2021,Revised on 27 May 2021,  
Accepted on 17 June 2021

DOI: 10.20959/wjpr20218-20744

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**Khushnuma F. Elavia****ABSTRACT**

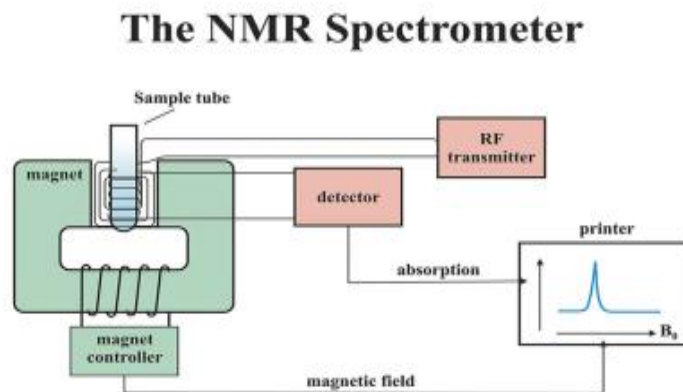
Nuclear Magnetic Resonance is one in all the foremost important analytical techniques that has been developed within past few decades. A broad variety of biological and nonbiological applications starting from a single cell to organs and tissues has been investigated through NMR. Many aspects of this method are still under analysis. This work is therefore meant to provide basic principles, concepts and unique applications of NMR in medical and dentistry.

**KEYWORDS:** Nuclear Magnetic Resonance Spectroscopy, Dentistry.**INTRODUCTION**

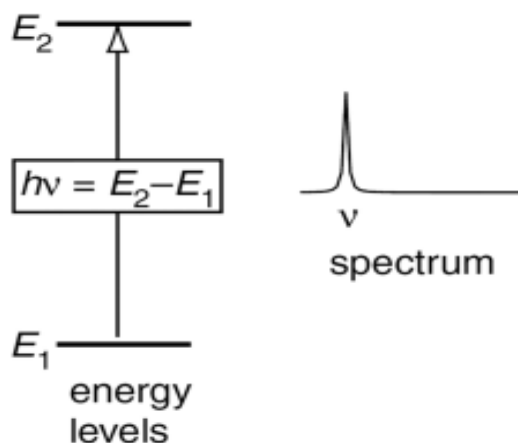
The electromagnetic spectra have been regularly utilized in the field of medication and dentistry to distinguish irregularities, but this detection tools causes danger to the patients due to excessive radiations and may damage tissues and organs.<sup>[1]</sup> New analytical methods have been developed which can give the exact outcomes with insignificant potential harms to the body tissues. NMR is one of those analytical technique which was found in the year 1940.<sup>[2]</sup> The NMR utilizes the magnetic properties and is generally being utilised in Chemistry, Physics and Biological science. In dentistry, this method is prevalently helpful to investigate the design of indistinct glasses, dental concretes, bioactive glasses connections with oral tissues, to identify salivary metabolites to detect infection<sup>[3,4]</sup> and understanding the periodontal infections by gingival crevicular liquid biomarkers analysis.<sup>[5,6]</sup> It is mostly used to check the fluoridation of apatite surfaces in the tooth.<sup>[7]</sup> Hence this review article is therefore meant towards giving a general idea of NMR, its principles and its advantages and limitations. Moreover it also gives the general idea of the applications of NMR in the field of medicine and dentistry and other future applications of NMR in different fields.

### Principle of nmr

The general principle of NMR are the structural and the chemical composition of unlike substances can be resolved by their nuclei which have different magnetic fields. The general NMR spectrometer analyser utilizes a magnetic field and a detector to identify the changes. The potential of the external magnetic field causes electrically charged nucleus to move from lower energy level ( $E_1$ ) to higher energy level ( $E_2$ ) and the difference between  $E_1$  and  $E_2$  is designated as  $\Delta E$  which is dependent on the power of magnetic field and the size of the nuclear field moment.<sup>[8]</sup> The electromagnetic radiation attains the NMR signal with a frequency ( $\nu$ ) give rise to the nuclei to move to a higher energy level ( $E_1/E_2$ ). When this electromagnetic radiation is stopped, it causes the nuclei to relax and attains thermal equilibrium. This energy which is released from the nuclei is recorded in the form of spectra on the computer, and these spectra are exclusive for every nucleus and are equivalent to the energy levels between the two states ( $E_2/E_1$ ).<sup>[8]</sup>



**Fig. 1: Schematic presentation of a typical NMR.**



**Fig. 2: Transition between two energy levels ( $E_2$  and  $E_1$ ).<sup>[9]</sup>**

## **General terminologies of nmr**

### **Nuclear spin**

The protons and neutrons of an atom shows spin. In some materials, the protons and neutrons shows paired spin for example., carbon  $^{12}\text{C}$ , oxygen  $^{16}\text{O}$  and in these cases, they cancel each other causing the nucleus not to spin. In some materials, the number of protons and neutrons in an atom are unpaired, for example., in proton  $^1\text{H}$  and fluoride  $^{19}\text{F}$ .

### **Applied magnetic Field and The nuclear moment**

The spin of the protons and neutrons generates a magnetic moment in the nucleus of an atom. This magnetic moment may be towards the external magnetic field or away from it. The magnetic field is responsible for holding the differentiation in the energy levels.

### **Magnetic field strength**

NMR requires a magnetic field that is both solid and uniform. The magnetic field strength is estimated in Tesla or MHz. The NMR requires a reference nucleus to address the strength of the magnetic field.

### **Chemical shift**

The movement of the electrons generates a magnetic field in and around the nucleus. This magnetic field generated is different in the direction as compared with the outer magnetic field. Any change in the magnetic field causes a comparative change in the spectrum of the NMR. This amount of the shift is constrained essentially of the nucleus and nature of the motion of electrons in its surrounding atoms and molecules. This phenomenon is called Chemical Shift (CS).

### **Spin–Spin coupling**

The nuclei close to each other make an incident called spin–spin coupling (SS) due to the difference in nuclei's magnetic field direction. This direction could be either towards or opposite the magnetic field, causing the splitting of NMR signals.

### **Spin relaxation (sr)**

Spin relaxation is the rebound of energy levels to stability. This happens due to the deficiency of resonance signals with the progression of time after releasing the resonance frequency. There are two relaxation processes which allows the nuclear spin to comeback to steadiness, which are spin–lattice relaxation and spin–spin relaxation.<sup>[10]</sup>

**Advantages**

1. Noninvasiveness
2. Shortness of ionizing radiation
3. Adjustability
4. Full structural analysis

**Disadvantages**

1. Presence of high magnetic field surroundings is necessary.

**Applications in Medicines and Dentistry**

In the field of medicine, NMR provides the advantages of identifying pediatric tumors, hematomas, and other pathologies.<sup>[11]</sup> As the multiple sclerosis is a very difficult disease to recognize, NMR has become the major diagnostic device for the identification of multiple sclerosis.<sup>[12]</sup> CT scan images of the cranium are limited by artifacts, but this disadvantage does not happen with NMR. NMR is clearly triumphant in identifying breast cancer at a beginning stage. As per the radiologist at Cleveland, a mammogram cannot distinguish between small cancer and a spot, when there are various types of cysts in the breast; however, with NMR, the differentiation of cyst has become possible.<sup>[13]</sup> NMR method also gives good images of fatty tissues, and a large quantity of fat creates wonderful images. Moreover, the determination of vascular diseases is promising with the NMR<sup>[14]</sup> as it empowers the detailed structural analysis of the surfaces of blood vessels and their irregularities.

In the field of dentistry, the objective of the treatment is to safeguard common tissues and remake the loss tissues with the assistance of biomaterials. The dental biomaterials are being examined by many machines such as mechanical analyzer, physical testing, rheological testing, and biocompatibility testing. For that, MR spectroscopy is a wonder machine to understand top to bottom chemical reactions of materials fixing and their impact with tissues. Broad research on Gas Ionomer Cement (GIC), tar composites, dental bone concretes, and periodontal film materials has been led utilizing NMR spectroscopy. The cross-connecting of Al in the setting of GIC is exceptionally urgent, furthermore, upon concrete development, Al particles in the glass are filtered out from the surface layer of the glass, which is uncovered by strong state NMR spectroscopy.<sup>[15]</sup> A novel antimicrobial polymeric dental helpful material was tentatively combined to see the biocompatibility, strength, and remineralization property by NMR (<sup>1</sup>H-and <sup>13</sup>C-NMR) spectroscopy.<sup>[16]</sup> The progressions of proteomics in dentistry have gotten an insurgency the administration of oral sicknesses what's more,

examination of atomic changes during the reproduction or then again restoration of oral tissues (delicate and hard) with dental materials.<sup>[17]</sup> To notice the orthodontically incited outer apical root resorption biomarkers, Zhou et al examined the <sup>1</sup>H-NMR-based metabolomics and recognized the provocative metabolites from spit samples.<sup>[18]</sup> This investigation brings an significance of NMR spectroscopy in the field of clinical dentistry also, dental early determination. Another examination on salivary metabolomics has announced the distinguishing proof of a few metabolic marks from the control and sarcoidosis patients.<sup>[19]</sup> The noninvasive, simple, and minimal effort testing of the human spit pulled in it as an analytic oral liquid, and by these omic gadgets like NMR, more biomarkers can be explored.<sup>[20]</sup>

## CONCLUSION

Thinking about the likely benefits of the NMR strategy, it can be finished up with power that it has gotten a liked decision of procedure for any determination, treatment arranging, support of treatment and furthermore to see the conduct of unfamiliar materials association with the human body. NMR is still a developing innovation, and it is being expected that meager few disclosures are presently practically around the bend.

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