

Nuclear Magnetic Resonance in Teflon and Polystyrene

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Abstract- We observed that in an amorphous substance containing protons (Teflon, polystyrene), the energy of the high-frequency field is absorbed due to such transitions. In this case, there are two levels, the distance between which, in accordance with the formula $h\nu = 2\mu H$, corresponds to a frequency ν , approximately equal to 20 MHz, at our value of the magnetic field. Although at room temperature $\frac{h\nu}{kT} \approx 10^{-5}$, the difference in the populations of these two levels is very small, the number of nuclei participating in this process is so large that a measurable effect can be expected at thermal equilibrium.

Keywords: resonance, teflon, polystyrene, orientation, high-frequency, inductive, g-factor, proton.

1. INTRODUCTION

The phenomenon of nuclear magnetic resonance (NMR), discovered in 1945 by F. Bloch and E. Parcell, now Nobel laureates, formed the basis for the creation of a new type of spectroscopy, which in a very short time turned into one of the most informative methods for studying molecular structure and dynamics of molecules, intermolecular interactions, mechanisms of chemical reactions and quantitative analysis of substances in various states of aggregation.

Since 1953, when the first NMR spectrometers were released, the NMR technique has been continuously improved, the flow of research will grow like an avalanche, new and traditional fields of application in chemistry, physics, biology and medicine are emerging and expanding.

The exclusive role of the NMR method in chemical research is determined by the fact that it turns out to be a useful and often irreplaceable source of information at all stages of research - from the emission of the composition of complex reaction mixtures to the establishment of the structure and dynamic characteristics of complex compounds, the distribution of electron density in them and intermolecular interactions.

A modern educated chemist, in whatever field he works, must acquire a fairly large amount of knowledge about nuclear magnetic resonance. Therefore, the curriculum of all leading universities in the field of chemistry necessarily includes lecture courses at various levels on NMR spectroscopy.

The physical foundations of nuclear magnetic resonance spectroscopy are determined by the magnetic properties of atomic nuclei. The interaction of the magnetic moment of the nucleus with an external magnetic field leads, in accordance with the rules of quantum mechanics, to the diagram of nuclear energy levels, since the magnetic energy of the nucleus can take on only some discrete values, the so-called eigenvalues.

These eigenvalues of energy correspond to eigenstates - those states in which only an elementary particle can be. Using a high-frequency generator, it is possible to induce transitions between eigenstates on the energy level diagram.

In this way, it is possible to obtain a spectrum of a compound containing atoms with non-zero nuclear moments. These atoms include the ¹H proton, the ¹⁹F fluorine nucleus, the nitrogen isotopes ¹⁴N and ¹⁵N, as well as many others of interest from a chemical point of view. But the nucleus of carbon ¹²C, which is so important for organic chemistry, as well as all other nuclei with an even mass number and an even atomic number do not have magnetic moments. Therefore, it is possible to study by NMR only the ¹³C isotope, the natural content of which is only 1.1%.

Various aspects of the use of nuclear magnetic resonance for solving the problems of inorganic, organic and physical chemistry are provided by a very wide variety of experimental techniques, which puts NMR spectroscopy in a special position in relation to other spectral methods. In addition to the variety of physical NMR experiments, the widespread use of this method is also facilitated by a wide variety of magnetic nuclei that are important from a chemical point of view.

In addition to proton NMR spectroscopy, useful information for organic chemistry and biochemistry is provided by ¹⁹F, ¹³C, ¹⁵N and ³¹P NMR spectroscopy. These nuclei are also important for research in inorganic chemistry. In addition, NMR spectroscopy on the nuclei of many metals is of considerable interest. Spectral parameters, i.e. chemical shifts and spin-spin coupling constants, are molecular constants that are important to theoretical chemists.

Measurement of these constants makes it possible to check the reliability of quantum mechanical methods used to describe the electronic structure of molecules. Thus, today NMR spectroscopy is a necessary method for all areas of science, be it biology, chemistry and physics.

2. METHODS OF OBSERVING NMR SIGNALS

Methods for observing NMR signals can be divided into two groups: observation of stationary signals and non-stationary NMR signals [1,2]. When stationary NMR signals are observed, a sample of a substance is subjected to the simultaneous action of two perpendicularly oriented magnetic fields: strong constant \vec{H}_0 and weak high-frequency field \vec{H}_1 . When observing non-stationary signals, polarization of nuclear spins and signal indication, polarization of nuclear spins and indication of NMR signals are separated in time.

The application of the NMR method is mainly limited to studies of stable and long-lived nuclei. This is due to the fact that in order to obtain noticeable signals, the sample must contain a sufficient number of nuclei with a magnetic moment. For example, to register NMR signals from hydrogen nuclei in a liquid at an operating frequency of 100 MHz, 1–20 mg of a substance is required. To record spectra for other nuclei, the relative sensitivity is lower and more substance is required.

The amplitudes of the NMR signals are proportional to the magnetization \vec{M} , which, in turn, is determined by the strength of the constant magnetic field \vec{H}_0 ; therefore, the stronger the strength of the constant magnetic field \vec{H}_0 , the higher the sensitivity of the NMR spectrometer.

An important characteristic of an NMR spectrometer is its resolution, which characterizes the smallest distance between two spectral lines that can be recorded separately.

The resolution depends on the width of the observed signals and, usually in NMR spectroscopy, is defined as the ratio of the signal width at half maximum to the strength of a constant magnetic field $\Delta H/H_0$. The main factor that determines the resolution of an NMR spectrometer is the inhomogeneity of the constant magnetic field. To improve the uniformity of the field, a field correction is used with the help of special correction coils, the so-called PWM, which compensate for the magnetic field gradients in the sample volume.

Using various methods, NMR is observed in fields from 0.01 oersted to 50,000 oersted, respectively, at frequencies from 10 Hz to 200 MHz. In high and medium (over 500 oersted) fields, NMR is observed directly, and in weak magnetic fields, due to a decrease in the total magnetization, additional nuclear polarization is usually used: static, dynamic, or by means of optical pumping [2,5].

In the well-known method of magnetic resonance, which applies the magnetic moments of nuclei in molecular states, transitions occur between energy levels that correspond to different orientations of the nuclear spin in a strong constant magnetic field.

We observed that in a liquid substance containing protons (Teflon and polystyrene), the energy of the high-frequency field is absorbed due to such transitions. In this case, there are two levels, the distance between which, according to the formula $h\nu = 2\mu H$ corresponds to the frequency ν , approximately equal to 20 MHz, at our value of the magnetic field. Although at room temperature $\frac{h\nu}{kT} \approx 10^{-5}$, the difference in the populations of these two levels is very small, the number of nuclei involved in this process is so large that a measurable effect can be expected at thermal equilibrium.

The time it takes to establish thermal equilibrium between the spins and the lattice is crucial here. The difference in the level population is necessary for absorption. This follows from the relationship between absorption and stimulated emission. In addition, even in the case when the relaxation time is very short, the absorption of energy and the high-frequency field will more or less rapidly (depending on the intensity of the high-frequency field) lead to a leveling of the level populations.

Desiring to have a long relaxation time (several minutes), we used such a weak oscillating magnetic field that absorption lasted for a minute, regardless of the relaxation time, if thermal equilibrium had already been reached. The resonator was a short section of the coaxial line, the load of which was the capacitance of the final plate. It was tuned to resonate at approximately 20 MHz. Its entrance and exit were provided with communication loops.

The inductive part of the resonator cavity was filled with 7500 mm³ of Teflon and polystyrene, which was kept at room temperature during the experiment. The resonator was placed in the gap between the magnet. The high-frequency magnetic field in the cavity of the resonator was perpendicular to the direction of the constant field. The cavity output is phase and amplitude balanced with respect to the other part of the generator output. With a balanced high-frequency circuit, the constant magnetic field was slowly changed.

In this case, an extremely sharp peak of resonance absorption was observed. The reading of the output device at the absorption maximum was approximately several times higher than the magnitude of fluctuations associated with noise and frequency instability. The equipment diagram and the results are shown in Fig. 1.

2. RESULTS

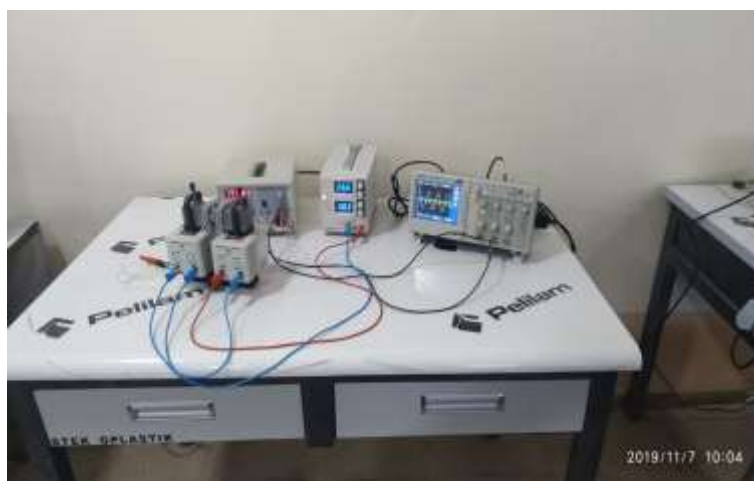
Determination of the g-factor of the proton of the Teflon and polystyrene molecules.

According to the resonance condition $h\nu = E_{k+1} - E_k = -g * \mu_n * B_0$ g – the factor of the proton in the glycerin molecule from the resonant frequency depending on the magnitude of the magnetic field.

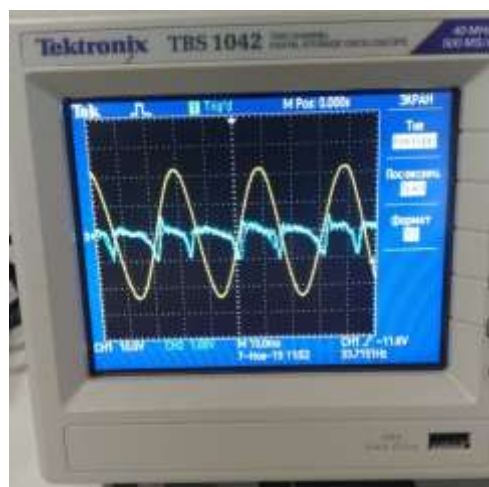
$$g = \frac{h}{\mu_n} * \frac{\nu}{B_0} \quad (1.1)$$

here, $\mu_n = 2.051 * 10^{-27} \frac{J}{T}$, $h = 6.626 * 10^{-34} Js$

The resonance occurred at a field of 850 mT and a frequency of 17.1236 MHz, in accordance with our preliminary rough calibration. We did not make an exact change in field and frequency. The magnitude of the magnetic moment of the proton, which follows from the given numbers, is 2.739 nuclear magnetons, which is in satisfactory agreement with the magnitude 2.7896 obtained by the molecular beam method.



a)



b)

Figure: 1. External view of the nuclear magnetic resonance equipment (a) and the results shown in the oscilloscope screen (b)

3. CONCLUSIONS

This method can be improved both in sensitivity and accuracy. In particular, it seems possible to increase the sensitivity by a factor of several hundred by changing the way the effect is detected. Apparently, the method can be used to accurately measure the magnetic moments (more precisely, gyromagnetic ratios) of the least abundant nuclei.

The method also allows one to study the interesting question of spin coupling. By the way, the method can be used to calibrate the magnetic field, since the equipment required for this purpose is very simple. The use of a high-frequency field by a rotating component would make it possible to expand the application of the method and determine the sign of the moment.

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