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Short Communication

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MEASURING NMR SPECTRA OF ZERO-SPIN NUCLEI

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ABSTRACT

NMR spectroscopy is one of the most powerful analytical methods. Along with its crucial in Chemistry, it has extremely wide applications in all science fields and medicine (MRI). With the current knowledge and technology, it is not possible to measure NMR spectra for zerospin nuclei. This is a severe limitation of the analytical method itself, and more important, to science, technology and medicine. In this communication we propose theoretical basis for activation of zero-spin nuclei, and consequently, enabling NMR spectra for compounds that contain them.

KEYWORDS: chiral center, polarized light, zero-spin nuclei, NMR spectroscopy, 12C, 13C.

INTRODUCTION: Nuclear magnetic resonance (NMR) spectroscopy is one of the most important analytical methods. Its uses are almost beyond count in all science disciplines. In medicine, magnetic resonance imaging (MRI) is top diagnostic tool. Despite all this, this spectroscopic method, and as a result all its uses, suffers a severe limitation in the current knowledge: it can not be applied and used for zero-spin nuclei.^[1]

To demonstrate the severity of this limitation, let us consider the case of an isolation (or laboratory synthesis) of a new natural product. Suppose that this compound has very low concentration in its source. Since the compound is new, it has to be characterized with several analytical methods, with at least hydrogen and carbon NMR spectra, on the top of them. As for ¹H, this is easy and possible since this isotope is the most abundant of hydrogen isotopes, around 99.99%, and it is non-zero spin, 1/2. As for carbon, the situation is entirely different. NMR spectrum can be measured only for ¹³C, also with nuclear spin of 1/2, but with natural

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abundance of 1.03%. The most abundant carbon isotope is ¹²C is 98.97%, but with a nucleus of zero-spin, I=0. This means that its NMR spectrum cannot be measured.

In this communication we propose that using polarized radiation instead of the non-polarized radiation normally used in this method, will activate zero-spin nuclei, induce spin split and enable NMR spectra measurement (figure 1).^[2]

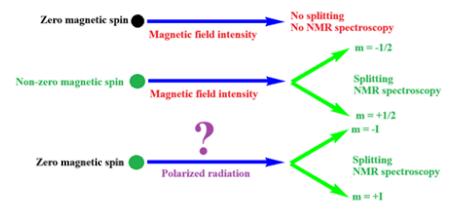


Figure 1: Proposed use of polarized radiation will activate zero-spin nuclei.

Scientific Justification: The interaction of light-matter is one of the most important phenomena in science and it had been utilized in numerous scientific fields. One of these fields is optical activity detection with polarized light. In its most classical occurrence, plane polarized light interacts with a chiral center and its plane rotate in a specific angle. The most common case is the interaction of plane polarized light with two compounds with asymmetrical carbon (chiral center, enantiomers) resulting opposite rotations. These rotations are named specific rotation (angles), and they can be experimentally measured and theoretically calculated. [4]

But the presence of a chiral center is neither sufficient nor necessary since chirality can emerge from other structures, as shown in figure 2.^[5,6]

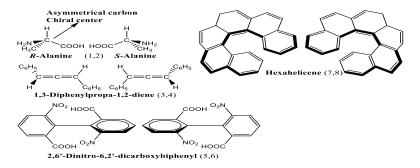


Figure 2: Optically active compounds, with and without chiral centers.

Moreover, it is now recognized that "new forces involve not only the chirality of the system on which they exert their mechanical action, but the chirality itself of the optical field that generate them".^[7] Finally, it was recently reported that polarized light can polarize spins of electrons in indium selenide.^[8]

In conclusion, considering the presented above properties of polarized light, there is a logically based probability that polarized light can activate zero-spin nuclei and enable measuring their NMR spectra and other uses like MRI.

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