Chemistry of nuclear spin isomers of symmetric molecules for new scientific and practical applications

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Unlike other types of molecular isomerism, nuclear spin isomerism is much less known. The existence of nuclear spin isomers of molecules (NSIM) has a quantum nature and is associated with the Pauli principle, which imposes strict restrictions on the total wave function of symmetric molecules. The most widely known nuclear spin isomers are those of the H_2 molecule, namely orthohydrogen (o-H_2) and parahydrogen (p-H_2), for which the total nuclear spin of two hydrogen atoms is equal to one (I=1) or zero (I=0), respectively. At the same time, other symmetric molecules also have two or more NSIM.

The unique properties of NSIM are of major interest in a broad range of scientific disciplines and practical applications. One of the most advanced areas of activity is the utilization of p-H_2 to achieve a dramatic NMR signal enhancement in the context of a range of the so-called nuclear spin hyperpolarization techniques. Unfortunately, efficient NSIM enrichment procedures currently exist for H_2 and D_2 only. This largely hinders the progress in extending the research to NSIM of other molecules. While several techniques for enrichment of NSIM of polyatomic molecules have been demonstrated, none is able to provide the quantities of enriched gases comparable to those available for H_2.

This presentation will demonstrate the wide range of potential applications of NSIM along with the results of the recent efforts to develop novel NSIM enrichment protocols. Parahydrogen-based NMR signal enhancement is very useful in the mechanistic studies of catalytic reactions, which now also covers heterogeneous hydrogenations catalyzed by a variety of types of solid catalysts, including supported metals, immobilized metal complexes, single-metal-atom and intermetallic catalysts, and more [1,2]. Hyperpolarization is also highly useful in the advanced studies of chemical reactions [3] and operating catalytic reactors [1] by NMR-based spectroscopic and imaging (MRI) techniques. Parahydrogen is widely explored to produce hyperpolarized biocompatible substances, including natural metabolites and drugs, for advanced biomedical imaging. The ortho:para NSIM ratio of gaseous molecules provides a glimpse at the past of the Universe in terms of the conditions of the formation of space objects some billions of years ago. The field is developing rapidly, and novel possibilities continue to emerge [4].

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