Parahydrogen as a tool to study chemical composition below the detection limit of magnetic resonance.

Indrek Reile

Indrek.reile@kbfi.ee

National Institute of Chemical Physics and Biophysics, Tallinn, Estonia

Parahydrogen hyperpolarization increases NMR signals by several orders of magnitude, allowing to detect analytes that occur below the limit of detection of conventional NMR. Such signal enhancement enables NMR in applications where the technique has traditionally been dismissed due to sensitivity reasons.

Compared to other hyperpolarization techniques (e.g., DNP), parahydrogen is less universal, enhancing only the signals of specific classes of analytes. It is, however, orders of magnitude less expensive and easier to set up, and therefore one of the more accessible ways to increase NMR sensitivity. We will demonstrate that this serves as a benefit in chemical analysis, from the analysis of relatively simple samples to highly complex biological mixtures. Combined with appropriate NMR detection schemes, hyperpolarization helps to analyze the otherwise undetectable portion of complex samples that consist of analytes in a wide range of concentrations.

To benefit from the sensitivity improvements on offer, we have developed proof of concept applications[1–3] that demonstrate the potential of parahydrogen hyperpolarization in chemical analysis. The talk will give an overview of the current application envelope and highlight the benefits of combining hyperpolarization with high, medium or low field[4] NMR instrumentation.

(1) Reimets, N.; Ausmees, K.; Vija, S.; Reile, I. *Anal. Chem.* **2021**, *93* (27), 9480–9485.

(2) Reimets, N.; Ausmees, K.; Reile, I. *J. Magn. Reson. Open* **2024**, 100171.

(3) Pais, H.; Reile, I.; Ausmees, K. *Anal. Chem.* **2025**.

(4) Urbańczyk, M.; Kork, K.; Ausmees, K.; Ratajczyk, T.; Reile, I. *Chem. Comm.* **2025**.