Case study

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Real-time Monitoring of Ortho to Para Hydrogen Conversions with Raman Spectroscopy

What is Raman spectroscopy?

Raman spectroscopy is an optical analysis technique that measures the vibrational properties of molecules. It has revolutionized process analysis with its high-resolution compositional data, linear response to concentration, non-destructive nature, ability to measure samples in real-time, and lack of a sampling system or carrier gases.

Fueling the future

Hydrogen is emerging as a promising new fuel source due to its potential to decarbonize various sectors, including transportation and energy production. Raman spectroscopy has become an ideal measurement technique for hydrogen production processes. This analytical method allows for the non-destructive analysis of molecular composition, providing insights into the efficiency and purity of hydrogen production methods. Researchers can optimize production processes by utilizing Raman spectroscopy, ensuring hydrogen's scalability and sustainability as a future fuel source.

Benefits of Raman spectroscopy

- Rich compositional information
- Quantitative and linear response
- Non-destructive
- No sample preparation
- Measuring all sample types
  - Solid/Powder/Slurry
  - Liquid/Gas
  - Heterogeneous samples
- Fast measurement times
  - Milliseconds to seconds – not minutes

Case study

The Massachusetts Institute of Technology (MIT) is one of the world's leading researchers in the conversion of ortho hydrogen to para hydrogen. Hydrogen is an important energy source, and its use is expanding rapidly, but it must be in liquid form for transportation and use. At 25 °C, molecular hydrogen comprises 75% ortho hydrogen and 25% para hydrogen. Hydrogen must be converted from the ortho form to the para form for energy efficiency and to prevent boiloff. MIT researchers use the MarqMetrix All-In-One and two interchangeable FlowCell sampling optics to monitor the ortho-to-para ratio and conversion rate under different conditions and catalysts.

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Requirements

- Solid-state, stable analyzer providing analysis in seconds
- High signal-to-noise ratio
- Excellent optical resolution
- Ability to collect spectra of hydrogen at 20 Kelvin in liquid form
- Method development using peak integration and normalization techniques

Results

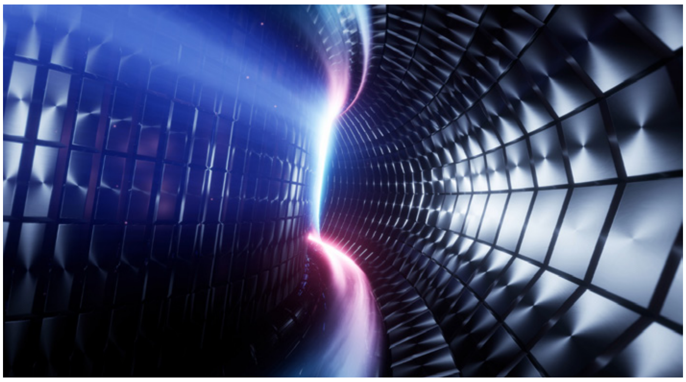
In this study, hydrogen gas was first cooled in a heat exchanger immersed in liquid nitrogen, then passed through a packed-bed reactor containing commercially available iron-based catalyst. This process facilitated the conversion of ortho-hydrogen to para-hydrogen, altering its equilibrium from 75% ortho at room temperature to 50%, effectively balancing the ortho-para ratio. Temperature, pressure, and flow rate were monitored and regulated. Downstream of the reactor, a Raman probe was deployed to measure the ortho-para hydrogen concentrations in real time, providing immediate insights into the efficiency of the conversion process.

The Thermo Scientific™ MarqMetrix™ All-In-One Process Raman Analyzer and Thermo Scientific™ MarqMetrix™ FlowCell™ Sampling Optic were successfully deployed to monitor the catalytic conversion of ortho to para hydrogen. This successful outcome was partly due to the FlowCell's ability to collect high-quality liquid and gas phase hydrogen spectra at cryogenic temperatures (77 to 20 Kelvin).

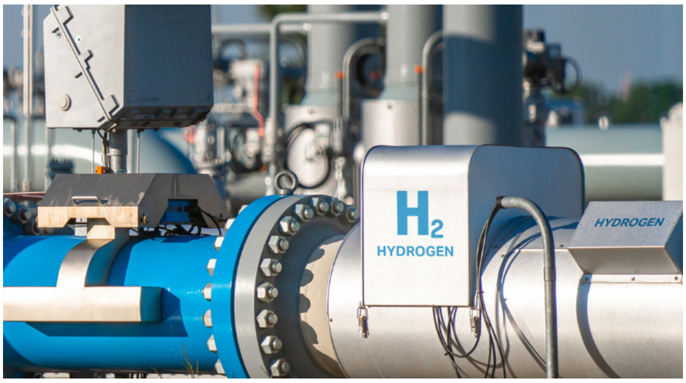
MarqMetrix FlowCell Sampling Optic is designed for easy integration into continuous flow applications.

Additional Clean Energy Applications

- Monitoring hydrogen/deuterium feed to fusion reactor for power generation



- Hydrogen blend into natural gas to reduce carbon footprint for power generation



- Measuring and controlling Sustainable Aviation Fuel (SAF) feedstock transformation

Learn more at **thermofisher.com/marqmetrixAIO**