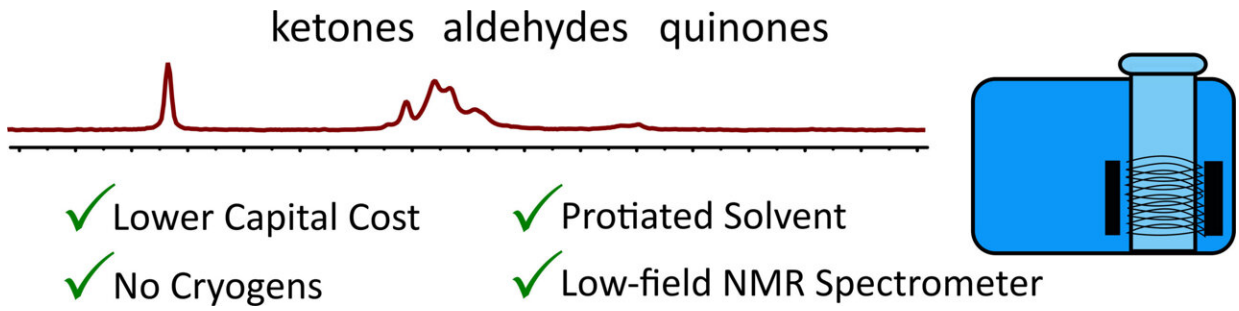
Exploring how benchtop NMR spectroscopy can accurately analyze pyrolysis oils

September 8 2023



Graphical Abstract. Simpler, cheaper, accurate: Low-field, or benchtop, nuclear magnetic resonance (NMR) spectrometers prove capable of quantitative analysis of pyrolysis oils from a range of lignocellulosic feedstocks. The NMR estimates of total carbonyl content compare favorably with titrations while the acquired spectra allow for the quantification of carbonyl groups such as ketones, aldehydes and quinones. Benchtop NMR spectrometers are cheaper than their superconducting counterparts and require neither cryogens nor deuteriated solvents. Credit: *ChemSusChem* (2023). DOI: 10.1002/cssc.202300625

A team of researchers at Aston University has demonstrated that benchtop spectrometers are capable of analyzing pyrolysis bio-oils just as well as far more expensive, high-field spectrometers.

Bio-oils resulting from the intense heating (pyrolysis) of industrial or agricultural by-products, are increasingly seen as potential alternatives to fossil fuels. But the stability and consequent treatment of these bio-oils

depends entirely on their composition; and since they are often mixtures of many dozens, or hundreds, of different compounds, analyzing such complex mixtures is not simple—or cheap.

Dr. Robert Evans, Senior Lecturer in Physical Chemistry at Aston University, explains, "The composition of any pyrolysis bio-oil is absolutely key to future use. For example if there are oxygen-containing chemicals in the oil, that will make the oil more corrosive and it will be more unstable. So in particular we need to know if carbonyl groups are present—where oxygen and carbon atoms are bonded together—as these can have a major impact."

A leading method of analysis is high-field nuclear magnetic resonance (NMR) spectroscopy, which gives a detailed breakdown of the identity and concentration of chemical species present in any sample. However these large high-field NMR spectrometry machines cost in the range of £600,000–£10million and require a supply of expensive cryogens and solvents, so are generally only found in the very biggest research facilities.

The team at Aston, led by Dr. Evans, set out to see if 'low-field', or benchtop, NMR spectrometers, could analyze pyrolysis oils well enough to produce the necessary detailed information. Benchtop NMR spectrometers use permanent magnets, which don't require cryogenic cooling, so cost much less to purchase and maintain.

However, using lower strength magnets comes at the cost of lower sensitivity and poorer resolution. While they can find some use as research instruments, they are also commonly found in teaching laboratories.

The study, carried out with collaborators at the University of Tennessee, tested pyrolysis oils produced from a number of different plants, and

compared the results from benchtop spectrometers to both high-field spectrometers and other methods of analysis. They found that the benchtop machine estimates compared favorably with titration analysis for overall carbonyl content, as well as matching high-field spectrometry for the specific identification of carbonyl groups such as ketones, aldehydes and quinones.

Dr. Evans said, "Despite the known limitations of benchtop spectrometers, a very similar quality of NMR data could be obtained for these samples, enough to accurately estimate concentrations of different classes of carbonyl-containing species. Using benchtop spectrometers will make NMR analysis of pyrolysis oils much simpler, cheaper, and more accessible to a wider range of different users."

"Quantitative Low-Field 19F NMR Analysis of Carbonyl Groups in Pyrolysis Oils" is published in *ChemSusChem*.

More information: Bridget Tang et al, Quantitative Low-Field 19F Nuclear Magnetic Resonance Analysis of Carbonyl Groups in Pyrolysis Oils, *ChemSusChem* (2023). DOI: 10.1002/cssc.202300625

Provided by Aston University

Citation: Exploring how benchtop NMR spectroscopy can accurately analyze pyrolysis oils (2023, September 8) retrieved 2 May 2024 from https://phys.org/news/2023-09-exploring-benchtop-nmr-spectroscopy-accurately.html

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