B144 An Analysis of Gaseous Mixture Adsorption by Nuclear Magnetic Resonance (NMR) Spectroscopy: Improving Our Understanding of Arson Debris Investigations

Christopher L. Suiter, PhD, National Institute of Standards and Technology, Boulder, CO 80305; Jason A. Widegren, PhD, Boulder, CO 80305; Megan Harries, BS, National Institute of Standards and Technology, Boulder, CO 80305; Kavita M. Jeerage, PhD, National Institute of Standards and Technology, Boulder, CO 80305; Tara Lovestead, PhD, National Institute of Standards and Technology, Boulder, CO 80305*

Learning Overview: After attending this presentation, attendees will learn how gas-phase NMR spectroscopy can provide valuable insight about the adsorbent properties of activated carbon by monitoring the real-time composition of gases in a sealed sample tube containing a carbon strip. Using this method, multiple compounds of interest can be detected and quantified simultaneously. In contrast to traditional approaches in which analytical techniques are used to determine what is desorbed after a solvent extraction of the carbon strip, this approach measures changes in the gas-phase composition to determine what has been adsorbed onto the carbon strip.

Impact on the Forensic Science Community: This presentation will impact the forensic science community by providing attendees with exposure to a new method that allows for monitoring the rate of compound adsorption, the impact of water vapor on adsorption, and the role, if any, of competitive adsorption effects between gas-phase mixtures and carbon strips. These findings have the potential to improve our understanding of gas-adsorbent interactions.

NMR spectroscopy is most often associated with investigations of molecules in the liquid-phase. While not common, NMR is occasionally applied for the study of gases.[1] Recently, the National Institute of Standards and Technology (Boulder, CO) research group developed a method for the quantitative analysis of low-pressure gas-phase mixtures by ^{1}H NMR spectroscopy.[2] With this method, low uncertainty composition determinations (<1%) can be made and data collected in a matter of minutes. Interestingly, during these experiments, unexpected adsorption between gas-phase mixtures and a Teflon® piston located inside of the sampling apparatus were observed. While inconvenient at the time, these findings led the research group to explore the possibility of measuring mixture adsorption for other systems of interest by NMR. Here, the original approach to measure gas-phase compositions in the presence of a carbon strip is extended in this work. Data for individual compounds and simple binary mixtures are presented that demonstrate the features of this technique and its potential impacts on the field of arson debris analysis; other problems of potential interest to the forensic community are discussed.

To conclude, NMR spectroscopy allows for low uncertainty composition determinations of gas-phase mixtures. Using this technique, questions related to the kinetics and competitive effects during gas-phase adsorption can be explored. This approach could improve our understanding of the underlying science of arson debris analysis and other topics in forensic science.

Reference(s):

1. Jameson, C.J. Gas-Phase NMR Spectroscopy. *Chem. Rev.* 1991. 91: p. 1375-1395.
2. Suiter, C.L., McClinden, M.O., Bruno, T.J., Widegren, J.A. Composition Determination of Low-Pressure Gas-Phase Mixtures by ^{1}H NMR Spectroscopy. *Anal. Chem.* 2019. **3**: p. 4429-4435.

NMR Spectroscopy, Arson Debris, Quantitative Analysis

*Presenting Author