

CHARACTERIZATION OF MIXTURES BY GAS CHROMATOGRAPHY COUPLED TO MOLECULAR ROTATIONAL SPECTROSCOPY

JUSTIN L. NEILL, ALEX MIKHONIN, MATT MUCKLE, *BrightSpec Labs, BrightSpec, Inc., Charlottesville, VA, USA*; MOHSEN TALEBI, *AZYP, LLC, Arlington, TX, USA*; NIMISHA THAKUR, M FAROOQ WAHAB, DANIEL W ARMSTRONG, *Department of Chemistry and Biochemistry, University of Texas at Arlington, Arlington, TX, USA*.

Gas chromatography is a gold-standard technique for analysis of mixtures of volatile compounds, and can be coupled to a range of detectors including many allowing for molecular identification (e.g., mass spectrometry). Recently, we have explored the use of molecular rotational resonance spectroscopy, with its extremely high sensitivity to subtle changes in molecular structure, as a rapid detector for gas chromatography effluents. Results from an initial study^a will be presented, where GC-MRR with a 75-110 GHz chirped-pulse millimeter-wave spectrometer was used to identify and quantitate mixtures, including co-eluting isotopologues and isotopomers which could not be resolved by other methods. Challenges for ongoing development, including data collection and interpretation, sensitivity optimization, and the column-spectrometer interface, will also be discussed.

^aD.W. Armstrong et al., *Angew. Chem. Int. Ed.* 2020, 59, 192-196