

SAMPLING REQUIREMENTS FOR MIXTURE ANALYSIS USING MOLECULAR ROTATIONAL RESONANCE SPECTROSCOPY

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Over the past few years, a number of studies have been performed that show the capability for gas-phase molecular rotational spectroscopy to perform quantitative mixture analysis. In particular, the ability of this technique to identify new compounds in a mixture on the basis of comparison to electronic structure theory is extremely powerful. For a number of reasons, however, the sample introduction and volatilization methods employed warrant new development. First, mixtures often contain components with different vapor pressures, and so care is required in extrapolating concentration information from observed signals.^a Additionally, operator-to-operator variability, measurement cycle time, and ease of use are factors that should be considered. We will discuss our efforts to develop sampling interfaces to enable routine quantitative mixture analysis using molecular rotational spectroscopy, as well as challenges that the field still faces.

^aC. West *et al.*, "Analysis of pear ester flavoring samples using broadband rotational spectroscopy," 2018 International Symposium on Molecular Spectroscopy, talk RH06.