New techniques for direct analysis of gas mixtures based on MRR spectroscopy.

Justin L Neill, Brent Harris, Matt T Muckle, Robin L Pulliam, Dave A McDaniel, Roger L Reynolds, Brooks H Pate

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We present new techniques for direct analysis of gas mixtures based on molecular rotational resonance (MRR), a new high resolution molecular spectroscopy technique for analytical chemistry applications. These measurements are enabled by the selectivity of pure rotational spectroscopy and the time resolved Fourier transform MRR design. While pure rotational spectroscopy is a well-established technique for structural characterization in academic research applications, the development of room-temperature, benchtop, Fourier transform instruments was only recently made feasible by advances in microwave and millimeter wave digital electronics. The pure rotational energy manifold of a gas phase molecule is governed by quantized angular momentum states dependent upon the moment of inertia. Any redistribution of mass in a molecule shifts the rotational spectrum, so isomers, conformers and isotopologues (with site specificity) are all distinguishable. The full bandwidth of the instrument, with ~10^5 distinct spectral resolution elements captures the highly resolved, periodic rotational fingerprints in the mixture and the components can be identified by simple library matching. For the unidentified (or ambiguous) lines in the spectrum, Fourier transform MRR can also be used to enhance the analysis through nutation dipole estimation, two-color pump-probe identity verification, and mass estimation measurements. Here we show the structural specificity, sensitivity, dynamic range, quantitation accuracy, and unknown identification capabilities of Fourier transform MRR spectroscopy.