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AUTOMATED MICROWAVE DOUBLE RESONANCE SPECTROSCOPY: A TOOL TO IDENTIFY AND CHARACTERIZE CHEMICAL COMPOUNDS

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Owing to its unparalleled structural specificity, rotational spectroscopy is a powerful technique to unambiguously identify and characterize volatile, polar molecules. We present here a new experimental approach, automated microwave double resonance (AMDOR) spectroscopy, to rapidly determine the rotational constants of these compounds without any *a priori* knowledge of elemental composition or molecular structure. This task is achieved by rapidly acquiring the classical (frequency vs. intensity) broadband spectrum of a molecule using chirped-pulse Fourier transform microwave (FTMW) spectroscopy, and subsequently analyzing it in near-real time using complementary cavity FTMW detection and double resonance. AMDOR measurements provide a unique "barcode" for each compound from which rotational constants can be extracted. To illustrate the power of this approach, AMDOR spectra of three aroma compounds — *trans*-cinnamaldehyde, α- and β-ionone — have been recorded and analyzed. The prospects to extend this approach to mixture characterization and purity assessment are described.