

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 polar molecules. We present here an experimental approach, automated microwave double resonance (AMDOR) spectroscopy, that allows to rapidly determine the rotational constants of such compounds without any a priori knowledge of elemental composition or molecular structure. This task is achieved by 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. Results obtained on the characterization of individual compounds and mixtures will be described.