STRATEGIES FOR INTERPRETING TWO DIMENSIONAL MICROWAVE SPECTRA

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Microwave spectroscopy can uniquely identify molecules because their rotational energy levels are sensitive to the three principal moments of inertia. However, a priori predictions of a molecule's structure have traditionally been required to enable efficient assignment of the rotational spectrum. Recently, automated microwave double resonance spectroscopy (AMDOR) has been employed to rapidly generate two dimensional spectra based on transitions that share a common rotational level, which may enable automated extraction of rotational constants without any prior estimates of molecular structure. Algorithms used to date for AMDOR have relied on making several initial assumptions about the nature of a subset of the linked transitions, followed by testing possible assignments by "brute force." In this talk, we will discuss new strategies for interpreting AMDOR spectra, using eugenol as a test case, as well as prospects for library-free, automated identification of the molecules in a volatile mixture.