STRATEGIES FOR COMPLEX MIXTURE ANALYSIS IN BROADBAND MICROWAVE SPECTROSCOPY.

AMANDA L. STEBER, JUSTIN L. NEILL, MATTHEW T. MUCKLE, AND BROOKS H. PATE, *Department of Chemistry, University of Virginia, McCormick Rd., P.O. Box 400319, Charlottesville, VA 22904*; D.F. PLUSQUELLIC, *Optical Technology Division, NIST, Gaithersburg, MD 20899-8441*; V. LATTANZI, S. SPEZZANO, AND M.C. MCCARTHY, *Harvard-Smithsonian Center for Astrophysics, 60 Garden St., Cambridge, MA 02138, and School of Engineering & Applied Sciences, Harvard University, 29 Oxford St., Cambridge MA 02138.*

Broadband microwave spectra often contain overlapping spectra from a large number of species in the sample mixture, whether in the study of conformational isomers, molecular complexes, reaction products from reactive molecular sources (*e.g.*, electrical discharge), or analysis of chemical mixtures. In these experiments, the identification of individual spectra in the full spectrum through pattern recognition becomes difficult when there is a high density of transitions. Strategies for extracting individual spectra from broadband measurements are discussed. Two approaches for microwave-microwave double resonance spectroscopy have been evaluated. One uses a transition-by-transition screening in a narrowband cavity spectrometer to identify an unknown spectrum and has a time advantage from the increased sensitivity of cavity spectroscopy. The second double-resonance approach uses a broadband spectral editing approach that gives a multiplex advantage in the detection. Both of these experimental techniques are combined with computer-aided assignment algorithms to make the spectral assignment in a minimum of double-resonance observations. The performance of spectral analysis solely using computer-aided assignment is also evaluated. The potential for fully automated spectral decomposition of the broadband spectrum of a complex mixture will be described.