THE ANALYSIS OF COMPLEX CHEMICAL MIXTURES BY BROADBAND ROTATIONAL SPECTROSCOPY

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Broadband rotational spectroscopy has several experimental advantages as a technique for the analysis of complex chemical mixtures without the need for chromatography to separate the distinct chemical species prior to analysis. The technique has high spectral resolution so that mixtures with a large number of components can be analyzed without spectral overlap, the frequency accuracy is excellent so that library spectra can be transferred between instruments, and the measurement has high dynamic range so that low level impurities can be detected in the presence of dominant species like the solvent in a direct-from-flask reaction mixture. It also has the special feature of a spectroscopic signature that is dependent on the molecular mass distribution so that isomers can be resolved – a problem that can be a challenge for the high-sensitivity analytical chemistry methods based on mass spectrometry. The problem of decomposing a measured spectrum into the individual rotational spectra of each different sample molecule is common to many applications of broadband rotational spectroscopy including reaction product screening in laboratory astrochemistry, the identification of different molecular clusters in the study of weakly bound complexes, and the analysis of chemical samples from a variety of chemistry fields including pharmaceutical science. In this talk we will discuss strategies that have been developed by the spectroscopy community to solve the problem of decomposing a measurement into its constituent spectra. These approaches include traditional analytical chemistry approaches like the creation of large chemical libraries. Instrumental methods that exploit broadband detection to implement efficient double-resonance methods will also be summarized. Two approaches that may deserve additional consideration in the future will also be discussed. One approach measures the spectrum as a function of a continuously variable external parameter and then uses computer algorithms to group transitions with similar parametric dependence as a way to separate the measurement into molecule-specific spectra. The second approach uses the fact that the Hamiltonian for rotational spectroscopy is known and that only certain patterns of transitions are consistent with it. An early example of this idea is the AUTOFIT routine. The possibility of extending this approach into a fully automated computer analysis of the spectrum will be considered.