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Complex Mixture Analysis Using Rotational Spectroscopy

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Owing to its very high intrinsic resolution, exceeding ppm levels in supersonic jet sources, rotational spectroscopy is a powerful analytical tool to analyze complex mixtures that consist of both familiar and exotic molecules. We present here an experimental method to rapidly sort rotational lines in broadband spectra and assign them to individual chemical compounds in the cm-band. This method combines a chirped-pulse FT microwave (CP-FTMW) spectrometer with follow-up analysis using an automated cavity FTMW spectrometer with double resonance (DR) capabilities. The CP-FTMW spectrum acts as a filter, identifying only those regions of frequency space that contain molecular signal, and discarding the vast majority of frequency space that is devoid of molecular information. With superior sensitivity and resolution per unit time, a cavity spectrometer is then used for follow-up assays on these bright spectral lines, to group transitions which share common characteristics, such as elemental composition, etc. These groups can be further partitioned into smaller sub-groups by exhaustive DR experiments whereby only those rotational lines that share a common energy level from the same molecule are linked together. From these series of measurements and assays, rotational transitions of multiple, individual chemical compounds can be empirically sorted and identified, without the need for any theoretical guidance or input. Significant automation greatly enhances the overall efficiency, enabling rapid, exhaustive testing with little oversight. Examples illustrating the power of this methodology for rapid analysis of broadband spectra will be presented.