

Chirped-Pulse Millimeter Wave Spectroscopy of EPA TCL Volatiles Mix 5 Standard: Advantages of Coherent, Pure Rotational Spectroscopy for Trace Level Volatile Mixture Analysis

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Conventional methods for gas mixture analysis do not address the need for multicomponent, trace level analysis of complex mixtures. Chirped-pulse millimeter wave spectroscopy has been recently introduced to the field molecular spectroscopy and promises new analytical capability for gas mixture analysis by utilizing the spectral signature of pure molecular rotation. Originally developed at the University of Virginia, chirped-pulse spectroscopy has become widely accepted by the chemical physics community as a highly sensitive, broadband technique for determining structure of molecules and complexes at microwave wavelengths. Recent advances in solid state terahertz devices and high-speed digital electronics have enabled the application of chirped-pulse spectroscopy to the millimeter wave spectrum where benchtop, room temperature measurements of small volatile organic compounds is highly favorable. The transformative advantages of chirped-pulse millimeter wave stem from the high resolution (0.0006 cm^{-1}), absolute specificity to molecular structure, and coherent, time domain measurements. As a result, high dynamic range composition analysis can be accomplished without chemical separation and with an essentially zero false positive rate. A suite of time domain measurements can be used to enhance the analysis with double resonance identity verification, mass estimation, and dipole estimation leading ultimately to library-free identification of unknown spectral carriers. Advantages and fundamentals of chirped-pulse spectroscopy are introduced and demonstrated on an Environmental Protection Agency standard mixture of Hydrofluorocarbons.