GAS ANALYSIS BY FOURIER TRANSFORM MM-WAVE SPECTROSCOPY

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Molecular rotational spectroscopy of low pressure, room temperature gases offers high chemical selectivity and sensitivity with the potential for a wide range of applications in gas analysis. A strength of the technique is the potential to identify molecules that have not been previously studied by rotational spectroscopy by comparing experimental results to predictions of the spectroscopic parameters from quantum chemistry so called library-free detection. The development of Fourier transform mm-wave spectrometers using high peak power (30 mW) active multiplier chain mm-wave sources brings new measurement capabilities to the analysis of complex gas mixtures. Strategies for gas analysis based on high-throughput mm-wave spectroscopy and arbitrary waveform generator driven mm-wave sources are described. Several new measurement capabilities come from the intrinsic time-domain measurement technique. High-sensitivity double-resonance measurements can be performed to speed the analysis of a complex gas sample containing several species. This technique uses a pi-pulse to selectively invert the population of two selected rotational energy levels and the effect of this excitation pulse on all other transitions in the spectrometer operating range is monitored using segmented chirped-pulse Fourier transform spectroscopy. This method can lead to automated determination of the molecular rotational constants. Rapid pulse duration scan experiments can be used to estimate the magnitude and direction of the dipole moment of the molecule from an unknown spectrum. Coherent pulse echo experiments, using the traditional Hahn sequence or two-color population recovery methods, can be used to determine the collisional relaxation rate of the unknown molecule. This rate determination improves the ability to estimate the mass of the unknown molecule from the determination of the Doppler dephasing rate. By performing a suite of automated, high-throughput measurements, there is the potential to determine the shape (via the rotational constant), electric properties (the dipole moments and its direction in the principal axis system), and the mass of the molecule to aid its identification.