Keysight Technologies

High-Speed Broadband Spectroscopy Measurements Advance Molecular Research

Application Note

KEYSIGHT TECHNOLOGIES

Introduction

Rotational spectroscopy has allowed the identification of hundreds of complex molecules and has enabled scientists to better understand the laws of the universe including the origins of life on Earth.

The rotational spectra of small molecules can be analyzed by optical methods in the infrared spectrum, however, the rotational transitions offer better resolution in mixtures and better specificity to molecular geometry.

The Keysight Technologies, Inc. next generation data conversion technologies have enabled the development of a new technique called segmented chirped pulse Fourier transform millimeter (CP-FTmmW) spectroscopy capable of extending spectroscopic measurements to other wavebands (millimeter/sub-millimeter and terahertz) to provide the precise rotational fingerprint of molecules.

Abstract

Spectroscopy measures the interaction between a sample and electromagnetic radiation (light). Light can be emitted (emission spectroscopy), absorbed (absorption spectroscopy) or scattered by a sample. Molecular spectroscopy can be used to determine the composition of a substance since a molecule's dynamics are uniquely affected by specific frequencies of light.

Molecular Rotational Resonance (MRR) spectroscopy, a form of molecular spectroscopy, enables the accurate identification of the molecular structure of gas phase molecules based on the change of angular momentum when interacting with the light field.

Recent improvements in electronic instrumentation have enabled the development of a chirped pulse Fourier transform millimeter-wave (CP-FTmmW) spectrometer capable of measuring the 260 – 295 GHz region of a rotational spectrum in a single data acquisition.

This document will describe how Keysight's data conversion technology, including the M8190A AXIe arbitrary waveform generator (AWG) and the U1084A high-speed PCIe digitizer with on-board signal processing, enable highly accurate rotational spectroscopy for the generation of a precise library of reference spectra and the investigative analysis of unknown species.

Application overview

Molecular Rotational Resonance (MRR) spectroscopy is a powerful tool for understanding the structure of molecules. It provides a non-invasive and non-destructive method of analysis and is useful in applications such as trace gas detection, atmospheric chemistry, and monitoring industrial processes.

However, the identification of certain types of molecules by MRR has been limited by conventional techniques, instrument detection limits, and the chemical properties of the molecules themselves.

In order to measure the rotational signature of molecules in highly diluted mediums, new methods such as broadband CP-FTmmW spectroscopy are needed.

High dynamic range, speed and time resolution are key features of test and measurement instruments required to perform segmented CP-FTmmW spectroscopy measurements. In addition, the availability of advanced, on-board, signal analysis features of digitizers can enable researchers to perform faster measurements.

Solution

High-speed test and measurement instruments are key components in a CP-FTmmW measurement system.

The Keysight M8190A 2-channel, AXIe, 12 GSa/s AWG is capable of creating high quality signals with 12-bit resolution and 5 GHz modulation bandwidth to provide the spectral purity of a best-in-class microwave synthesizer. The M8190A is housed in Keysight's M9502A 2-slot AXIe chassis with an extremely fast PCIe Gen 2 interface to a PC.

AWG sequencing provides a straightforward, highly adaptable platform for generating the unique chirp sequences, shown in Figure 2, necessary for fast reference library creation that is essential for the broad adaptation of rotational spectroscopy in promising new pharmaceutical applications.

The Keysight U1084A Acqiris high-speed digitizer is a dual channel, 8-bit PCIe digitizer card with up to 4 GS/s sampling. The U1084A features an on-board, high-speed, field programmable gate array (FPGA) for real-time processing of acquired data such as on-the-fly signal averaging, peak detection and simultaneous acquisition and readout (SAR).

Signal averaging drives the sensitivity of CP-FTmmW measurements. The combination of the U1084A's deep on-board signal averaging and SAR capabilities increases data throughput and reduces the time to generate reference spectra from days to minutes.

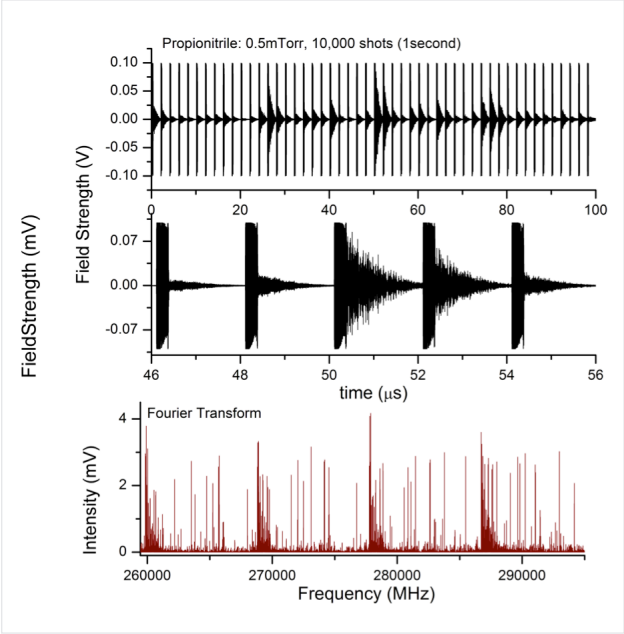

Figure 2. Time domain, segmented molecular emission traced out on the U1084A digitizer and zoomed in for clarity. The bottom plot is the library spectrum.

Solution details

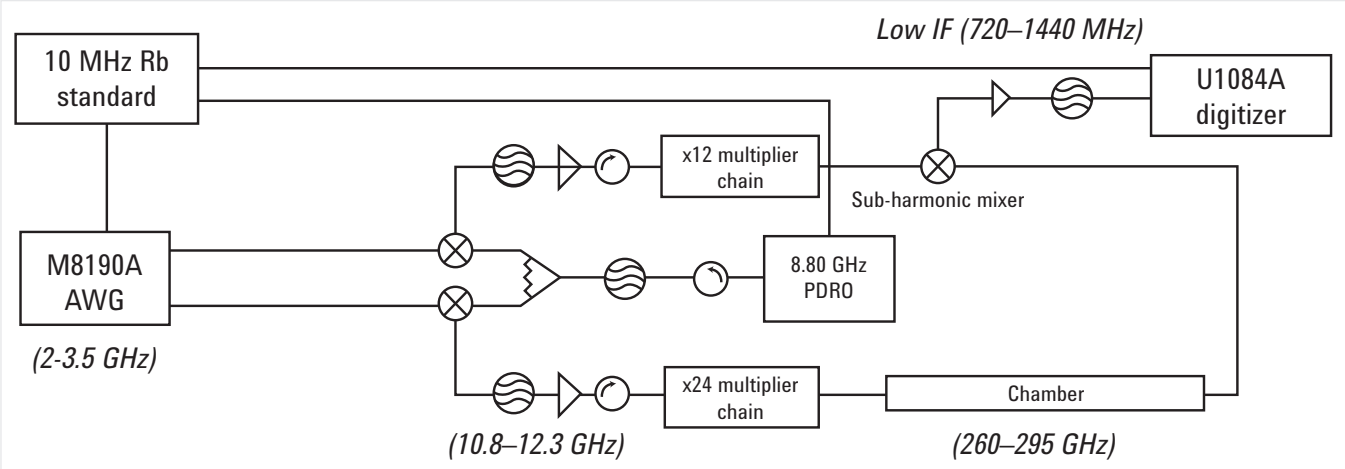

Figure 3. Block diagram of CP-FTmmW spectrometer

A CP-FTmmW spectrometer consists of three main sections: signal generation and amplification, molecule interaction, and signal capture and analysis. Figure 3 illustrates a block diagram of a CP-FTmmW spectrometer. Note that all components are synchronized to a 10 MHz external reference clock, a requirement for subsequent averaging of signals in the time-domain.

Keysight's M8190A 2-channel, AXIe, 12 GSa/s AWG is capable of creating a chirped pulse that provides frequency sweeps in segments from 2 to 3.5 GHz each in 250 ns with 12-bit resolution. By generating a very fast linear sweep of frequencies; it is possible to generate an envelope of radiation spanning a wide frequency range with maximum spectral purity that can be used to excite rotational transitions in a gas sample.

The chirped pulse is then up converted to a microwave frequency in the 10–12 GHz range by mixing it with an 8.8 GHz phase-locked dielectric resonator oscillator (PLDRO). The up converted signal is multiplied to a millimeter wave frequency range between 260-295 GHz, amplified and broadcast into the molecular interaction section where it polarizes the sample.

The resulting coherent molecular emission, or FID signal, is down converted to a low intermediate frequency (720-1440 MHz) for digitization. Keysight's U1084A 2-channel, PCIe, 8-bit, high-speed digitizer, can capture a FID signal at 4 GS/s.

On-board signal averaging in the time-domain is performed on more than 1 million coherent FID signal acquisitions to improve the signal-to-noise ratio by approximately 1000 and simultaneously readout the highest quality signal for further analysis. A fast Fourier transform of the averaged signals produces the frequency-domain spectrum of the molecular emission to reveal the molecular structure of the gas sample.

In summary, Keysight's data conversion technology has enabled the development of new molecular research techniques based on CP-FTmmW spectroscopy that allow researchers to make faster measurements at millimeter-wave frequencies than were previously possible with conventional spectroscopy techniques.

Figure 4. U1084A Acqiris PCIe digitizer

Figure 5. M8190A 2-channel AXIe AWG

Ordering information

Model	Description
M8190A	Arbitrary waveform generator, 2 channels
U1084FA-001-AVG	Acqiris PCIe digitizer with on-board signal processing
M9502A	AXIe chassis: 2-slot with integrated system module
Related products	
M9505A	AXIe chassis: 5-slot with integrated system module
M9536a	AXIe embedded controller

Want to know more?

Product information
www.keysight.com/find/m8190a
www.keysight.com/find/u1084a
www.keysight.com/find/m9502a

Software information

Supported operating systems	Microsoft Windows 7 (32/64-bit) Microsoft Windows Vista (32/64-bit) Linux
Keysight IO libraries	Includes: VISA Libraries, Keysight Connection Expert, IO Monitor

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