Reprogrammable multi-species gas monitors based on Fourier transform millimeter-wave spectroscopy

Molecular Rotational Spectroscopy for Chemical Analysis

Pure rotational spectroscopy in the millimeter and submillimeter is a well established technique in academic research settings, with seven decades of instrument development anchoring the BrightSpec technology. Spectrometers for molecular rotational spectroscopy combine the operational simplicity of Fourier transform infrared spectroscopy (FT-IR) with the sensitive and selective chemical analysis capabilities of mass spectrometry. The innovations pioneered by BrightSpec scientists have enabled the first commercially viable, general-use millimeter wave rotational spectrometers for gas monitoring and mixture analysis. Some of the key features of BrightSpec rotational spectrometers are:

- **High chemical selectivity** without separation, even in a complex mixture.
- **Breadth of application**: Any molecule with a permanent dipole moment has a rotational spectrum and so can be monitored with BrightSpec instruments.
- **Simplicity of operation**: The light field is generated digitally, so no lasers to maintain, and no routine calibration is needed.
- **Speed**: Full mixture analysis can be performed in less than a second.
- **Dynamic range** exceeding $10^5$ for identifying trace components.
- **Intensity precision** is 0.1% or better, enabling precise quantification of abundances and detection of small changes.

Molecules of Interest

Some of the molecules identified in market discovery discussions that will be sensitively characterized by the BrightSpec technique are:

- Ammonia
- Carbon monoxide
- NO and NO$_2$
- Nitrous oxide
- Formaldehyde
- Hydrogen cyanide
- Difluoromethane (CF$_2$H$_2$) and other halocarbons
- Phosphine
- Chlorine dioxide and other EPA-regulated compounds
- Acrolein
- Ethanol
- And many more...

BrightSpec Science Sensitivity, Dynamic Range, & Signal Linearity

The performance of the Targeted Band instrument is demonstrated with the detection of very rare isotopologues of OCS. Abundant isotopes are seen in only a second or less of data acquisition, while weak isotopes at the $<10^{-6}$ mole fraction level can be seen within a few minutes. The experiment control is totally customizable - monitor as many or as few lines as you like. The acquisition time can also be allocated arbitrarily in order to utilize instrument time efficiently: spend only a few seconds checking on your primary components, then use the rest on the trace species.

Instrument response is linear over 5 orders of magnitude.

Monitoring of 4 isotopologues of OCS. Strong components are seen within 1 second, trace isotopologues require a few minutes of signal averaging to lower the noise floor.
Coherent Pulse Sequences for High-Confidence Assignments

In complex mixtures, frequency overlaps between lines of different species can occasionally happen. In order to eliminate the possibility of a misidentification, BrightSpec instruments are equipped to perform two-color coherence measurements, based on the principles of multidimensional NMR. One pulse (the pump) alters the quantum state populations, and the second (the probe) measures that perturbation. An increase in the probe signal with the pump pulse on confirms with complete certainty that the detected transition is due to the molecule of interest.

Transitions that share a quantum level are discovered through the use of two-color coherent spectroscopy.

Two lines nearly coincident in frequency: the left one is resonant with the “pump” transition and is modulated, the right one is not resonant and is left alone.

Isotopic Analysis

Because of the intensity reproducibility of the digitally generated light field, BrightSpec instruments can monitor isotopic ratios for anomalies. This is enabled by linear performance over a wide dynamic range. The rotational spectrum is set by the mass distribution, so inequivalent isotopologues (for example, $^{15}\text{N}^{14}\text{NO}$ and $^{14}\text{N}^{15}\text{NO}$) have completely distinct spectra and are easily distinguished, enabling complete site specificity. The frequency shifts with substitution are dependent on the molecular structure and are accurately predicted from theory.

Other Product Configurations

Enantiomeric Excess Analyzer

BrightSpec is in the process of developing an instrument that uses a handed electric field to measure enantiomeric excesses and absolute chiralities in the gas phase with high accuracy, without the need for a chiral solvent. Because of the high spectral resolution of rotational spectroscopy, these determinations can be made in a complex mixture without need for a separation step, as with other BrightSpec instruments.

Dedicated Single-Molecule Sensors

For customer needs where only a single molecule - for example, water or ammonia - needs to be monitored, we can make specialized sensors with significantly lower cost and footprint.

Company Background

BrightSpec aims to address currently unmet needs in a variety of analytical markets. We fill critical gaps between FT-IR, GC/MS, GC-FID, NMR, and cavity ring-down spectroscopy techniques. In 2012, as a result of participating in the NSF-sponsored iCorps Lean Launchpad program, we personally interviewed over 100 would-be end users of our products. In early 2013, BrightSpec completed Series A financing to hire a team of four physical chemists, build out a dedicated 2,400 sq. ft. lab and instrument assembly space, and fund initial operations.

BrightSpec Products and Services

BrightSpec brings a major new advance in gas sensors: the first commercial Pure Rotational Spectrometer platform for manufacturing process control and environmental monitoring. We quantify and qualify, in nearly real-time, trace levels of volatile organic compounds (VOCs) in a complex mixture, without the need for chromatographic separation.

Gas Sensing and Monitoring

For applications where ultralow detection limits are desired on one or a few molecular species, the BrightSpec Targeted Band Spectrometer can reach ppb-to-ppt detection limits in seconds to minutes of measurement time. If the analysis needs change, BrightSpec can reprogram the instrument in software to enable the detection of a new set of target molecules. This instrument has the ability to discriminate between isomers, conformers, and isotopes, and to determine the enantiomeric excess for chiral samples.

Gas Analysis and Identification of Unknowns

BrightSpec ONE is a broadband survey spectrometer that performs full characterization of gas samples. After sample injection and characterization, the spectrometer returns a list of all known species detected in the sample, along with their concentrations in the mixture. Other lines attributed to unknown species can be identified through BrightSpec exclusive coherent technologies. No prior knowledge about the mixture composition is required.