HORIBA Scientific

THz-Raman[®] Spectroscopy Benchtop Module



TR-BENCH (with optional vial/tablet holder)

Features

- Compact, patented¹ optical design with integrated high power single frequency laser source
- Interchangeable sample interface vial/tablet holder, steerable open beam, or contact probe tip
- Fiber coupled output enables easy interface to a wide range of spectrometers
- Fast collection of THz-Raman[®] spectra from 5cm⁻¹ to > 3000 cm¹ (150 GHz to 90 THz)
- Simultaneous Stokes and anti-Stokes signals improve SNR while providing inherent calibration reference
- Can be added on to an existing Raman system or spectrometer, or incorporated into a complete turnkey system
- Available at 532 nm, 785 nm, and 850 nm excitation wavelengths

Applications

- Polymorph identification and analysis
- Crystallization Studies and Reaction Monitoring
- Trace detection and source attribution of explosives/hazmats/drugs
- Structural studies of nano- and bio-materials, photovoltaics, and semiconductors
- Forensics, archeology, mineralogy



¹ Patents #8,184,285 and 7,986,407

THz-Raman® – The "Structural Fingerprint" of Raman

HORIBA's new **THz-Raman® Spectroscopy Modules** extend the range of traditional Raman spectroscopy into the terahertz/low-frequency regime, exploring the same range of energy transitions as terahertz spectroscopy – without limiting the ability to measure the fingerprint region. This region reveals a new "Structural Fingerprint" to complement the traditional "Chemical Fingerprint" of Raman, enabling **simultaneous analysis of both molecular structure and chemical composition in one instrument** for advanced materials characterization.

See What You've Been Missing – More Data, Better Sensitivity & Reliability

Clear real-time differentiation of structural attributes of the material enables clear identification and analysis of polymorphs, raw material sources, defects and contamination, crystal formation, phase monitoring and synthesis methods.

One Sample, One System, One Answer

In-situ, real-time measurement of both composition and structural analysis eliminates the need for multiple samples and instruments, lowering capital, training and maintenance costs.

Benefits

- Both chemical composition + molecular structure from one Raman measurement
- In-situ, real-time structural monitoring + chemical analysis
- Higher SNR with inherent calibration reference
- Faster, more comprehensive and reliable measurements
- Compact, easy to use, and adaptable to existing Raman systems and spectrometers



THz-Raman Fingerprint Region -200 - 200cm⁻¹ 200 - 2,000+ cm⁻¹

Full Raman spectrum of the pharmaceutical carbamazepine showing both the THz-Raman "Structural Fingerprint" and traditional "Chemical Fingerprint" regions. Note higher intensity and symmetry of THz-Raman signals.

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THz-Raman® Real-time monitoring of both structure and composition

THz-Raman[®] measurements capture low-frequency lattice and phonon modes that are manifested by both inter- and intra-molecular vibrations. These modes are highly responsive to changes in molecular structure and can be used to monitor structural changes caused by polymorphic or isomeric shifts, lattice defects, contaminants, and changes in phase or crystallinity. The examples below show how THz-Raman can be used to observe polymorphic shifts, distinguish phase transformations, characterize cocrystalline mixtures, or determine synthetic pathways.



Polymorph Detection

Polymorphic forms and hydrates of pharmaceuticals can easily be distinguished in raw materials analysis, finished goods, process monitoring, and QC applications.



Crystal Monitoring

Monitoring the presence or formation of cocrystals is also improved using THz-Raman spectra. The figure above shows the clearly recognizable peak shifts that occur when cocrystals are formed in a mixture of caffeine and 2-Benzoic acid.



Synthetic Pathway Analysis - Explosives Forensics

Multiple samples of ETN (Erythritol Tetranitrate), representing systematic variations of ingredients and preparation routes, show distinctive differences.



Phase Monitoring

Phase changes of sulfur observed when heated from room temp.(a) to 95.2°C (β) and then to the melting point of 115.21°C (λ). Note the clearly recognizable changes in peak location, shape, and magnitude in the THz-Raman region. Crystalline phases result in sharp peaks, which broaden and dissipate as the sulfur liquefies.

Sample Interface Accessories



Vial / Tablet Sample Holder

Steerable Collimated Beam Mount

Adjustable Probe Tip Mount

Fixed SwageLok Probe Tip Mount

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A variety of sample interface accessories enable the TR-PROBE and TR-BENCH to be easily configured to match a broad range of applications. The Vial/Cuvette Sample Holder incorporates an adjustable steering mirror, interchangeable focusing lens, and safety shutter. Immersion or Contact probe tips may be mounted with either a fixed SwageLok mount or, for longer probes that may need alignment, an adjustable tip/tilt probe mount. And the Steerable Collimated Beam Mount allows for projection and steering of the collimated output beam with precision alignment and interchangeable focusing optics, for applications requiring long-range collection paths.

THz-Raman® TR-BENCH Module Specifications:

Parameter	Units		Specification			
Wavelength	nm	532	785	850	976	
Power at sample port (min)	mW	25 to 2501	60	60	300	
Physical Dimensions (W x D x H) ²	in			12" x 10" x 3"		

¹ Specify power level at time of order

² Base unit only, does not include sample accessory

Spectrometer³:

	iHR320 Spectrometer ³	iHR550 Spectrometer ³
Spectral Range (typical)	-3400 cm ¹ to +3400 cm ¹	-3400 cm ¹ to +3400 cm ¹
Spectral Resolution	0.8 cm ¹ or greater	0.5 cm ⁻¹ or greater
Computer Interface	USB	USB

³ With 1200g/mm grating

System Description and Configurations:

All **TR-Series** THz-Raman[®] modules are ultra-compact and simple to connect via fiber to any HORIBA spectrometer or Raman system. The patented **SureBlock[™]** ultra-narrow-band Volume Holographic Grating (VHG) filters precisely block *only* the Rayleigh excitation with >OD 8 attenuation, enabling simultaneous capture of both Stokes and anti-Stokes signals. A high-power, wavelength-stabilized, ASE-free single-frequency laser source is precisely matched to the filters to assure maximum throughput and exceptional attenuation of the excitation source.

The **TR-BENCH** is configured for benchtop use and offers a variety of sample interface accessories, including a convenient vial/tablet/NMR tube holder, a steerable collimated beam, and immersion or contact probe tips for fast, easy measurements (see sample options on previous page). The system also comes with a standard cage mounting plate (centered on the collimated output beam) to allow for customized collection optics or easy integration into a customized system. The TR-BENCH includes a stabilized 532 nm, 785 nm, 850 nm, or 976 nm laser source, ASE and notch filters, and optional circular polarization.



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THz-Raman®

Additional Applications



Pharmaceutical Applications

Key challenges for the pharmaceutical industry include polymorph identification, reaction monitoring, raw material quality control, and counterfeit detection. THz-Raman[®] reveals "structural fingerprints" that can rapidly differentiate polymorphs, isomers, cocrystals, and other structural variations of substances and compounds.



Semiconductor and Nanomaterials

Graphene and carbon nanotubes are just two of the many nanomaterials that exhibit strong low-frequency signals. For graphene, THz-Raman[®] analysis can determine the number of monolayers, and for carbon nanotubes, the diameter of the structure. Differences in structural characteristics and defects in crystals can also be detected.



Industrial and Petrochemical

THz-Raman[®] delivers additional sensitivity and information about molecular structure to control processes, improve yields, and monitor crystallization or structural transformation during formulation of chemicals and polymers.



Explosives Detection, Forensics and Source Attribution

THz-Raman[®] goes beyond chemical detection to reveal a "structural fingerprint" that can be attributed to specific ingredients, methods of manufacture, and storage/handling of many popular homemade explosive (HME) materials, revealing clues about how and where they were formulated.



Crystallization and Reaction Monitoring

Low-frequency THz-Raman[®] signals undergo clear, rapid shifts corresponding to changes in molecular structure, enabling highly sensitive, real-time monitoring of crystal form, phase, or structural transformations.



Gas Sensing

Rotational modes of gases such as oxygen provide signal intensities up to 10x those in the fingerprint region. Stokes/anti-Stokes ratios can also be used for remote sensing of temperatures in gases, plasmas, liquids and solids.



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