THz-Raman® Spectroscopy Probe

**Features**

- Robust, sealed optical design with broad operating temperature range for use in demanding environments
- Fiber coupled high power CleanLine™ ASE-free laser source
- Interchangeable sample interface - probe tip, cuvette/tablet holder, transmission Raman adapter, microscope adapter, or steerable open beam
- Fiber coupled output enables easy interface to a wide range of spectrometers Fast collection of THz-Raman® spectra from 5cm⁻¹ to >3000cm⁻¹ (150GHz to 90THz)
- 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 as a complete custom-configured system
- Available at 532nm, 785nm, 808nm, 976nm and 1064nm excitation wavelengths

**Applications**

- Crystallization and Reaction Monitoring
- In-situ Polymorph identification and analysis
- Tablet and bulk materials measurements (with Transmission Raman accessory)
- Trace detection and source attribution of explosives/hazmat/drugs
- Structural studies of nano- and bio- materials, photovoltaics, and semiconductors
- Forensics, archeology, mineralogy

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**THz-Raman® – The “Structural Fingerprint” of Raman**

Ondax's patented THz-Raman® Spectroscopy Systems 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 & contamination, crystal formation, phase monitoring and synthesis methods.

**One Sample, One System, One Answer**

In-situ, real-time measurement of both chemical composition and molecular structure 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
- Interchangeable sample interface
- Compact, easy to use, and adaptable to existing Raman systems

**Carbamazepine (Form 3)**

Full Raman spectrum of the pharmaceutical compound Carbamazepine showing both the THz-Raman “Structural Fingerprint” and traditional “Chemical Fingerprint” regions. Note higher intensity and symmetry of THz-Raman signals.

1 Patents #8,184,285, 7,986,407, 9,599,565 and 9,587,983
Real-time, in-situ 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 example below shows how THz-Raman can be used as a real-time monitor of polymorphic changes in Theophylline.

Reaction Monitoring of Polymorphism

The figure below shows low frequency spectra of anhydrous theophylline (Form II) before and after its transformation into a flocculated slurry (monohydrate, Form M). Spectra collected at the start and finish (T=2s red and T=200s blue) show the disappearance of peaks at 20, 35 and 85 cm⁻¹ in the anhydrous spectrum and the appearance of a new peak at 96 cm⁻¹ in the spectrum of the monohydrate.

The waterfall plot (above right) shows the transformation from Form II to Form M is complete in approximately 100 seconds. The spectrum of the suspended solids was resolved from the broad underlying boson peak and the profile shown above. The time profile shown at right was then generated, which shows the disappearance of Form II (red) and the appearance of Form M (blue).

Data courtesy Clairet Scientific, Ltd.

Sample Interface Accessories

A variety of sample interface accessories enable the TR-PROBE to be easily configured to match a broad range of applications. Immersion or Contact probe tips may be mounted with either a fixed SwageLok mount or an adjustable tip/tilt probe mount. The Vial/Tablet Sample Holder incorporates an adjustable steering mirror, interchangeable focusing lens, and safety shutter. 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. A new Transmission Raman adapter enables bulk sample testing of tablets and vials, and the Microscope Adapter provides a mounting interface for scientific-grade microscopes, including and in/out optical switch.
THz-Raman® TR-PROBE Specifications:

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Units</th>
<th>Specification</th>
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<tbody>
<tr>
<td>Wavelength</td>
<td>nm</td>
<td>532 785 808 976 1064</td>
</tr>
<tr>
<td>Power at sample port (min)</td>
<td>mW</td>
<td>25 to 250 300 300 300 300</td>
</tr>
<tr>
<td>Physical Dimensions (W x L x H)</td>
<td>in</td>
<td>3&quot; x 8.5&quot; x 2.3&quot;</td>
</tr>
</tbody>
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1 Specify power level at time of order
2 Probe head only, does not include sample accessory

Spectrometer3:

<table>
<thead>
<tr>
<th>Spectrometer Type</th>
<th>Fixed Grating Spectrometer</th>
<th>Tunable Grating Spectrometer</th>
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</thead>
<tbody>
<tr>
<td>Spectral Range (typical)</td>
<td>-200 cm⁻¹ to +2200 cm⁻¹</td>
<td>400-1100 nm (w/Si Detector)</td>
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<tr>
<td>Spectral Resolution</td>
<td>2.5 cm⁻¹ to 4 cm⁻¹</td>
<td>0.7 cm⁻¹ or greater</td>
</tr>
<tr>
<td>Computer Interface</td>
<td>USB</td>
<td>USB</td>
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</table>

3 Spectrometer selection and specifications will be determined by application requirements and options ordered

System Description and Configurations:

All TR-Series THz-Raman® modules are ultra-compact and simple to connect via fiber to almost any spectrometer or Raman system. Our patented SureBlock™ ultra-narrow-band Volume Holographic Grating (VHG) filters precisely block only the Rayleigh excitation with >OD8 attenuation, enabling simultaneous capture of both Stokes and anti-Stokes signals, including the entire fingerprint region. 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. Systems are available at 532nm, 785nm, 808nm, 976nm and 1064nm.

The TR-PROBE is a compact, robust THz-Raman® probe that enables in-situ reaction or process monitoring, and can also be flexibly configured with a variety of sample interface accessories, including immersion or contact probe tips, a convenient vial/tablet holder, a Transmission Raman adapter, a microscope mount, or a steerable non-contact optic (see options below). A separate CleanLine™ laser provides ASE-free excitation via a multimode fiber, enabling the probe to operate in harsher environments where electrical connections are not permitted.

The TR-BENCH is configured for benchtop use and offers a similar range of interchangeable sample interface accessories holder for fast, easy measurements. The system also comes with a dovetail flange to allow any of our sample interface accessories to be interchangeably mounted. Options include circular polarization and a dual-port/dual polarization output for simultaneous measurement of both S and P polarizations.

The TR-MICRO mounts directly to a broad range of popular microscope platforms and micro-Raman systems, and can be easily switched in and out of the optical path. Linear polarization is standard, circular polarization is optional.
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, co-crystals, and other structural variations of substances and compounds.

**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 home-made explosive (HME) materials, revealing clues about how and where they were formulated.

**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.

**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.

**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.

**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.