

GENERAL MICROTECHNOLOGY & PHOTONICS

RANAAN Coen SPECTROSCOPY

OH

SPECTROMETERS ACCESSORIES SUBSYSTEMS COMPLETE SOLUTIONS



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What is Raman Spectroscopy?

Collecting Raman signal is like listening to the whisper of a molecule. One in every million incident laser photons scatters from the vibrational energy levels of the molecule, yielding information about the way it stretches and bends. Individually, the spectral lines detected speak to structure and composition, while collectively they can reveal identity.

Raman spectroscopy is being used to characterize materials for authentication, forensics, process and guality control, and is employed as a portable method of rapidly "fingerprinting" materials of interest for first responders - including explosives, narcotics and unknown chemicals.

Ocean Optics has been fueling the Raman revolution for 20 years, offering a diverse family of modular and turnkey systems. Designed for maximum performance in a compact, cost-effective footprint, our products let you take the power of Raman spectroscopy wherever you need to go.



Research and Science

Anti-Counterfeit

Security

Biotechnology

Advantages of Raman Spectroscopy

- No sample preparation needed
- Compatible with aqueous samples, unlike FT-IR
- Rapid identification of materials via matching to spectral libraries
- Non-destructive sampling of liquids, solids, gels and surfaces
- Non-invasive measurement through bags, vials and cuvettes

Modular vs. Turnkey Systems

Modular systems let you think outside the box, customizing everything from laser wavelength to measurement speed for your unique needs. Integrated systems lock in Raman shift range and resolution, as well as excitation wavelength - perfect for a well-defined application.

Raman Spectroscopy for OEMs

We have solutions for every step of the product development process, from proof of concept in the lab to compact and cost-effective production units in volume. In choosing a single, versatile partner, you get consistent support and applications knowledge, even as your product needs change.

www.gmp.ch



Selecting a Raman Spectroscopy System

Designing a Raman spectroscopy system is a balancing act. Signal and fluorescence background compete in selecting the excitation laser wavelength, while Raman shift range and resolution must be balanced at the detector. The application itself determines the needed performance and optimum laser wavelength. A turnkey, integrated system can work well for well-understood applications, but when the operating wavelength is unique or a specific resolution is required, a modular system is a better choice.



Modular Systems Flexible and configurable for unique needs

Our modular products allow you to build the exact Raman system you need, while maintaining the flexibility to change and optimize components as your needs evolve.

A modular system begins with your choice of excitation laser, typically routed to the sample with a specialized Raman probe (free-space coupling is also possible). Scattered Raman light is collected by the same probe and routed to a spectrometer that is configured with the sensitivity, optical resolution and Raman shift range needed for your application. We even offer sample holders to facilitate measurement of liquids in cuvettes and vials.

Modular systems offer the most value and flexibility when getting started with a new Raman application, and transition easily into OEM systems. Our modular Raman components include multiple lasers, probes and user-configurable spectrometers to suit almost any need.



| | Modular Systems | | | | |
|--------------------------------|---|--|--|--------|---------|
| Excitation Laser | Multiple options: 532 nm, 785 nm, custom Pag | | | Page 6 | |
| Raman Probe | Multiple options: general purpose, immersion, process Page | | | Page 6 | rie, |
| Spectrometer | QE Pro Series | Ventana Series | Maya2000 Pro Series | | |
| Features | Maximum flexibilityWeak Raman signals | High throughput Fast measurements | Cost effective Broad spectral range | Page 4 | .or ng |
| Preconfigured Spectrometers | QE <i>Pro</i> -Raman (785 nm) | Ventana-532-Raman Ventana-785-Raman Ventana-785L-Raman | Maya2000 Pro-NIR (785 nm, 808 nm) | | uration |
| Custom Configuration | User-defined spectral range Changeable slits to optimize resolution | None | User-defined spectral range and resolution | | |



Modular Spectrometers

Raman spectroscopy requires detection that balances sensitivity and signal to noise with resolution. These spectrometers do so elegantly, each optimized for a particular type of application. Our Maya2000 Pro and QE *Pro* spectrometers can be custom-configured to your exact excitation wavelength, resolution, range and sensitivity requirements, while their preconfigured versions and our Ventana series are ideal for 532 nm or 785 nm excitation.



Maya2000 Pro

The Maya2000 Pro is a good general purpose, configurable spectrometer for Raman, combining a low stray light optical design with an uncooled back-thinned FFT-CCD detector for enhanced sensitivity that is valuepriced. High quantum efficiency in the NIR makes it an excellent choice for long-wavelength Raman.

QE Pro

This high sensitivity, configurable spectrometer yields the highest quality Raman spectra, both in resolution and signal to noise. Designed with gold-coated mirrors and a back-thinned FFT-CCD detector cooled to -15 °C, it offers a low noise floor even at long integration times. Its ability to deliver sharp peaks from very weak Raman signals makes it an excellent choice when your exact application needs are undefined.

Ventana Series

The Ventana series of preconfigured spectrometers are designed specifically for Raman spectroscopy. By using a volume phase grating and a lower f/# than our other spectrometers (f/1.3 vs. f/4), they deliver higher throughput for fast measurements. This is further enhanced by control of the detector temperature at +15 °C, keeping the noise floor consistent for applications at short integration times.

Preconfigured Spectrometers for 785 nm Raman Excitation

| | Maya2000 Pro-NIR | QE Pro-Raman | Ventana-785-Raman |
|---|---------------------------|--|---|
| Raman Shift Range* | 0 – 4200 cm ⁻¹ | 0 – 2800 cm ⁻¹ | 200 – 2000 cm ⁻¹ |
| Resolution @ 810 nm* | 13 cm-1 | 11 cm ⁻¹ | 10 cm ⁻¹ |
| Detector Temperature | Unregulated | –15 °C | +15 °C |
| S:N Ratio | 450:1 | 1000:1 | 550:1 |
| Alternate Configurations | Custom Maya2000 Pro | Custom QE <i>Pro</i> with user-changeable slits | 532 nm version |
| Broad range High NIR efficiency General purpose | | Weak signals Long integration times Highest quality data | Low f/# (high throughput) Fast measurements |

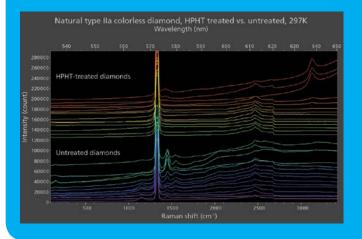
*Based on 785 nm excitation

$\overset{}{\bigstar}$

Application Note: *HPHT Treated Diamonds*

Natural diamond is quickly discriminated from imitation using the presence of a

strong Raman peak at 1332 cm⁻¹, easily authenticating a stone's value. Identifying high-pressure, high-temperature (HPHT) treated diamonds requires more subtle analysis.



Technical Note: Comparing Noise and S:N Ratio



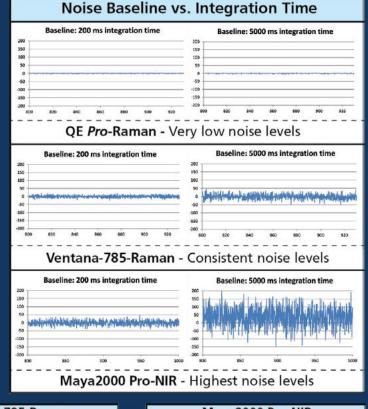
The noise inherent in a Raman spectroscopy system is one of the largest factors impacting data quality and ability to resolve peaks. Measurement

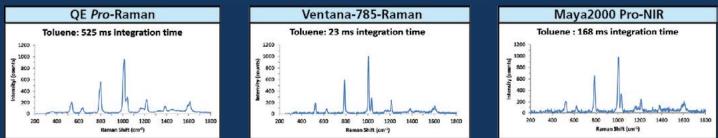
of baseline noise for our modular Raman spectrometers at 200 ms and 5000 ms integration time demonstrates the differences in temperature control of the detectors and how they impact noise. *See graphs on right.*

We looked at spectra of toluene acquired at low laser power to compare the overall sensitivity and S:N ratio of the spectrometers. The Ventana yields a good quality spectrum in just 23 ms, and is ideal for fast measurements. The Maya2000 Pro-NIR spectrum at 168 ms is noisier, but adequate for many stronger Raman signals, at a lower price point. It is the QE *Pro*-Raman, however, that truly shines, with a very clean, low-noise spectrum at a much longer 525 ms, making it the spectrometer of choice for long integration time measurement of weak Raman signals. HPHT treatment is used to alter near-worthless brown and gray type IIa diamonds to near-colorless by annealing the strain present within the diamond lattice. HPHT-processed diamonds cost 45-65% less than their untreated counterparts, but are not always labeled as such, creating the potential for fraud.

Fortunately, photoluminescence spectroscopy contains clues indicating HPHT-treatment, conveniently performed using a modular QE *Pro* Raman system. Both photoluminescence and Raman peaks appear in the spectrum, excited by a 532 nm laser. The strong 1332 cm⁻¹ peak and weaker ~2200– 2700 cm⁻¹ band are Raman scattering, while the smaller peaks at 536, 567, 576, ~580, 587 and 596 nm (upper scale) are photoluminescence peaks typical of defects in natural diamonds. HPHT treatment removes most of these peaks, leaving only nitrogenvacancy defect peaks at 576 and 637 nm in some samples.

Image courtesy of Foral Design Ltd. See www.gemmoraman.com for instrument details.





Excitation Lasers Benchtop and OEM modules



A laser with excellent stability and spectral purity yields a clean, high quality Raman spectrum. Our multimode 532 nm and 785 nm excitation lasers use innovative stabilization and thermoelectric cooling to lock wavelength, making them as reliable as they are easy to use. Their high power, narrow linewidth and side mode suppression of greater than 40 dB results in extremely high signal-to-noise ratio Raman spectra.

Our 532 nm and 785 nm turnkey models have integrated laser drives and TEC control electronics, with the ability to adjust laser drive current from the front panel or remotely. The compact 532 nm subsystem version is ideal for integration into OEM packages, and is designed to be driven remotely.

Other wavelengths are available upon request.

Raman Probes Maximum sampling flexibility



Probes can collect Raman spectra from solids, surfaces, liquids or powders. Designed to focus <1 cm from their tip, they also allow spectra to be collected non-invasively through vials and bags.

Our high quality fiber-coupled probes include designs for general purpose, immersion and process use. Filtering at the probe tip blocks fluorescence generated in the fiber by the laser, and transmits only Stokes scattered light back to the spectrometer, eliminating the need for additional filtering.

- Deep blocking of Rayleigh scatter from the sample (OD>8)
- Broad spectral range of operation (250-3900 cm⁻¹)
- Manual safety shutter on general purpose probes
- 532 nm or 785 nm; other wavelengths upon request

Customized Solutions for OEMs Made-to-order Volume Application Solutions

Many OEM customers begin with a modular system for proof-of-concept testing on the benchtop. This allows them to define their needs exactly while collecting high quality data to build analytical models or spectral libraries. Once the application and baseline performance requirements are well understood, we work together to design a customized system that delivers maximum value. Sampling optics and the excitation laser can also be customized using free-space optics to improve optical efficiency, reduce system size, and measure lower Raman shifts.

Our broad product range and ability to custom-engineer components, subassemblies and complete systems allow you to transition smoothly from concept to volume. We understand your application needs from start to finish, taking you from lab to launch and beyond!





Integrated Systems

Turnkey operation for targeted applications

Integrated systems are a convenient solution for applications where your excitation wavelength, Raman shift range, and resolution needs are known and unlikely to change. They operate at the more common laser wavelengths, and use free-space optics in place of fiber optic probes. This can improve sensitivity, and enables unique sampling modes like raster orbital scanning (ROS) or micros-copy. Our integrated systems outshine the competition in performance and value, from benchtop systems for the lab to a handheld unit for the field.

| | | | Integrated Systems | | |
|-----------------|-----|---|--|---|---------------|
| | | Benchtop | | Handheld | |
| Features | | Spatial averagingLower average power | Specific location High efficiency | Field useMatching libraries | - |
| | 532 | ✓ | ✓ ✓ | | Fixed |
| Excitation | 638 | ✓ | | | |
| Wavelength | 785 | \checkmark | ✓ | ✓ | Co |
| (nm) | 808 | ✓ | | | nfi |
| System | | | | | Configuration |
| | | IDRaman reader | IDRaman micro | IDRaman mini | |
| Applications | | SERS and tagging Delicate samples Pharmaceuticals Research and QA labs | Carbon nanotubes Semiconductors Life sciences Art and forensics | Explosives, narcotics Materials inspection Anti-counterfeiting Process lines | |
| Product Details | | Page 8 | Page 9 | Page 10 | |

Anti-counterfeiting of Fuels

As governments crack down on fuel adulteration and fraud, fuel marking becomes a more important component of fuel control programs to deter illegal activity. Authenticators can use SERS (surface enhanced Raman spectroscopy) to rapidly test for the presence and concentration of silver colloid markers added to fuels at the refinery; this helps to determine the fuel's integrity and origin. Customization of the system in a field-portable case with drop-in sample ports permits on-site testing, while GPS, barcode scanning and remote data return features instantly transfer location-specific data to a central server.





IDRaman reader Benchtop measurement of liquids and solids

The IDRaman reader delivers all the performance of a larger, more expensive system, converting seamlessly between solid and liquid samples. Enabled with raster orbital scanning (ROS), it offers low background, high resolution and sensitive measurements of non-uniform and inhomogeneous samples in a footprint that moves easily around the lab.

An adjustable focus sample holder accommodates vials and cuvettes for study of liquids. The source knob on the laser unit allows you to switch easily to measurement of solid samples, SERS substrates and surfaces in the space below the unit, with a user-exchangeable lens for adjustment of focal length.

Choose from 5 High-performance Systems:

| Systems Available | Raman Shift Range | Resolution |
|----------------------|-----------------------------|---------------------|
| IDRaman reader 532 | 200 – 3200 cm ⁻¹ | 7 cm ⁻¹ |
| IDRaman reader 638 | 200 – 2000 cm ⁻¹ | 8 cm ⁻¹ |
| IDRaman reader 785 | 200 – 3200 cm ⁻¹ | 10 cm ⁻¹ |
| IDRaman reader 785HR | 200 – 2000 cm ⁻¹ | 4 cm ⁻¹ |
| IDRaman reader 808 | 200 – 2000 cm ⁻¹ | 4 cm ⁻¹ |

- Turnkey operation for the lab or process line
- Sample from bottom of vial for small volumes
- Optional side measurement of cuvettes or vials
- Downward facing lens for solid samples





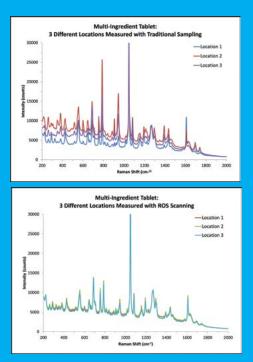
Application Note: *ROS Probes Inhomogeneous Pharmaceuticals*

Raster orbital scanning (ROS) is a sampling technique that moves the laser in a daisy-like pattern over the sample surface to capture a larger area. By measuring multicomponent antacid tablets at several different locations with and without ROS, we can see how inhomogeneity impacts Raman spectra.

Without ROS, the spectra taken at three fixed locations on the tablet show varying background and relative peak intensities. A number of the weaker peaks, possibly due to ingredients in lower concentration, are just barely resolved in some scans, while ratios for even the strongest peaks vary considerably with point of measurement.

With ROS activated, the background is lower on average, since more Ramanactive compounds are seen compared to autofluorescing components. All peaks present in any non-ROS scan appear in every ROS scan, regardless of position of measurement. The ROS scans also have more consistent peak ratios, which is key to accurate spectral library matching.

By scanning the sample in an orbital raster pattern, ROS obtains data that is equivalent to the average of roughly 20 fixed position scans. This increased measurement reproducibility greatly improves the quality of Raman data obtained when looking at complex, inhomogeneous or non-uniform mixtures, as well as components present in low concentration, regardless of the point of measurement.





IDRaman micro Image specific locations with high efficiency

The IDRaman micro delivers spatial resolution, excellent collection efficiency, and high quality spectra at a fraction of the size and cost of a traditional Raman microscope. The superior OneFocus optical system performs Raman measurement and imaging in a single focal plane for optimum sensitivity and ease of use. Created for maximum flexibility, this system is ideal for the research or QA/QC lab. It offers considerably better signal to noise than fiber-coupled systems of comparable cost, and better resolution of weak and closely spaced peaks.

- High quality imaging of sample
- Lever switches measurement from stage to vial
- Sample from bottom of vial for small volumes
- Interchangeable objectives
- Micro or macro view of a specific location

Choose from 3 High-performance Systems:

| Systems Available | Resolution | Raman Shift Range |
|---------------------|---------------------|-----------------------------|
| IDRaman micro 532 | 7 cm ⁻¹ | 200 – 3200 cm ⁻¹ |
| IDRaman micro 785 | 10 cm ⁻¹ | 200 – 3200 cm ⁻¹ |
| IDRaman micro 785HR | 4 cm ⁻¹ | 200 – 2000 cm ⁻¹ |





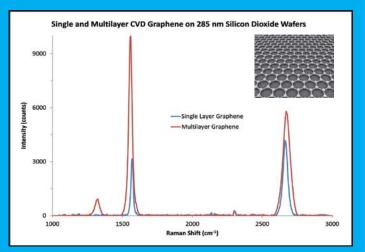
Application Note: Understanding Graphene

Carbon nanomaterials have unique properties, and are finding new applications in aerospace, catalysis, sensors and electronics. Raman spectroscopy is ideal for rapid, non-destructive characterization.

Graphene exhibits several characteristic Raman peaks. The G band observed at ~1580 cm⁻¹ indicates the number of graphene layers, shifting to lower energy as layer thickness increases. The G' band at ~2700 cm⁻¹ can also be used, albeit via a more complex relationship. The D band at ~1350 cm⁻¹ arises from defects in the material (amorphous carbon), and acts as a marker of purity.

To assess the ability of the IDRaman micro 532 to study graphene, we measured both single and multilayer samples from 200-3200 cm⁻¹. We used the Clean Peak function in OceanView software to remove background, capturing high quality data from all three bands of interest.

A shift of ~12 cm⁻¹ between the single and multilayer samples was observed for the G band, while the G' band width broadened from 39 cm⁻¹ for the single layer sample to 60 cm⁻¹ for the ~4 layer sample. As compared to the 7 cm⁻¹ resolution of system, this demonstrates system performance that is fully capable of building an accurate model of layer thickness. Additionally, the appearance of the D band with an intensity of ~930 counts for the multilayer system shows dynamic range that is more than adequate for assessment of defect levels.





IDRaman mini Handheld material identification in the field

The IDRaman mini is designed for rapid identification of materials, from field measurements of chemical and explosive agents to counterfeit detection and authentication analysis. Its ability to be used in harsh and demanding environments is well suited to quality assurance and verification of incoming materials, as well as in-line process monitoring.

Purchase Our Extensive Spectral Libraries, or Quickly Build Your Own.

This compact, rugged unit is the ultimate in portability. The resistive touch screen with intuitive interface makes it easy to operate, while self-calibration and advanced spectral processing to remove fluorescence background ensure highly confident material identification. Raster orbital sampling (ROS) with a 785 nm laser is used to collect accurate data even from inhomogeneous samples, without ignition or damage.

- Point and shoot operation
- Measure solids or liquids (vials)
- Real time library matching

System Available

IDRaman mini 785

- Spectral comparison and confidence factor
- Use our libraries, or build your own
- Long battery life: 1 day from charge





Software and Libraries

Raman Shift Range

400 - 2300 cm⁻¹

The IDRaman mini is preloaded with a library of 30 common Raman spectra to get you started. Also available are the spectra for over 9,000 additional compounds, including explosives and related materials. These spectra can be unlocked, by subset, upon purchase of the appropriate licensing codes. Here are some of the options:

Resolution

~13 cm⁻¹

- Chemicals: alkanes; alcohols and phenols; esters, lactones and anhydrides; aldehydes and ketones; hydrocarbons; sulfur and phosphorous compounds; solvents
- Applications: biochemical analysis; forensics; hazardous and toxic chemicals identification
- Industries: cosmetics and fragrances; flavors and food additives; pesticides; dyes and pigments



Tech Tip: Choosing a Raman Excitation Wavelength

Raman signal is proportional to $1/\lambda^4$ of the excitation wavelength. While this makes it tempting to use a short wavelength laser, autofluorescence generated in the sample can easily degrade signal to noise and make Raman peaks difficult to resolve. Organic samples are particularly prone to autofluorescence, driving

excitation to red or NIR wavelengths (660-830 nm). The effect is much less pronounced for inorganic materials, including carbon nanotubes and fullerenes, more commonly studied with 532 nm excitation.

Autofluorescence can be avoided entirely by moving to 1064 nm excitation, where our NIRQuest series of spectrometers can be used for detection.



High-Performance SERS Substrates

In Surface Enhanced Raman Spectroscopy (SERS), analytes are adsorbed on a silver or gold surface prior to analysis, boosting the Raman signal intensity by millions of times. The use of solid state substrates for SERS allows

ppb-level detection of chemical and biological materials in the field, as well as pharmaceuticals, explosives and tags for anti-counterfeiting. Visit our website to see a full list of analytes tested and the detection limit achieved using an Ocean Optics Raman spectroscopy system.

Trace Detection Made Affordable

Most SERS substrates are fabricated using expensive lithography techniques and are not reusable, making cost a deterrent for mainstream applications. Ocean Optics substrates offer better performance than the competition at a fraction of the price by using inkjet printing to precisely deposit special nanoparticle ink on paper, which is then immobilized on glass slides.

Dependable Peak Ratios

Our SERS substrates offer the same enhanced sensitivity when used with all our Raman systems and spectrometers. Though peak intensity varies from substrate to substrate, peak ratio repeatability is very good, typically 5% or less. This allows the substrates to be used both quantitatively and to determine presence vs. absence of the analyte.

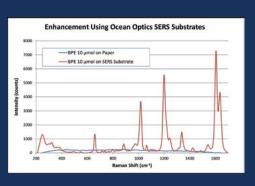
Tech Tip: ROS Helps SERS Hit the Spot

ROS is an advantage when performing SERS, as it samples hotspots of the analyte on the substrate more frequently relative to the background. The result is improved sensitivity and lower detection limits, with less chance of damage to the substrate due to heating. Selectivity is also increased, while fluorescence effects decrease, since characteristic peaks stand out more clearly against the background, even at high laser power. Other advantage of ROS include:

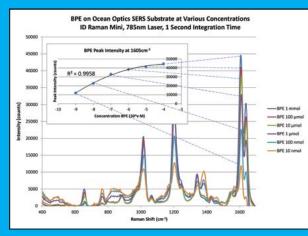
• Protects delicate samples like dyes and pigments, and avoids ignition in explosives

Helps prevent misidentification due to damage of the sample by high laser power





Application Note: *Quantitative SERS Detects Picomoles*



SERS unlocks the power of Raman spectroscopy and opens the door to quantitative measurements of trace materials. It can be used to screen imported food for the presence of banned fungicides and pesticides, or to analyze residues from surfaces for narcotics or explosives. It can also detect tracers added to high-value materials for authentication; absence of the tags clearly identifies counterfeit material, while reduced concentration indicates adulteration via dilution or introduction of substitute materials.

To assess the applicability of our SERS substrates to quantitative applications in the field, we looked at varying concentrations of BPE (1,2-Bis(4-pyridyl)ethylene) using the IDRaman mini handheld system.

Measurements of peak height at a Raman shift of 1605 cm⁻¹ as a function of concentration resulted in a high-quality polynomial fit capable of accurately quantifying an unknown sample. It should also be noted that this quantitative model covered a 6-octave concentration range, from mmol to nmol levels, and could likely be extended to an even lower limit of detection (LOD).



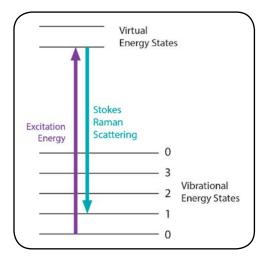
Tech Tip: Calculating Raman Shift

Raman spectroscopy studies vibrational energy levels by looking at the energy difference between laser light incident on the sample and the rare photon scattered

inelastically via the Raman effect. This energy difference, known as the Raman shift, is reported in energy units called wavenumbers (cm⁻¹).

The following equation shows how to calculate a Raman shift, Δv , in cm⁻¹ using the laser wavelength (λ_0) and a Raman peak wavelength (λ_x) in nm:

$$\Delta v_{x}(cm^{-1}) = \left(\frac{1}{\lambda_{0}(nm)} - \frac{1}{\lambda_{x}(nm)}\right) \times \left(\frac{10^{7} (nm)}{cm}\right)$$



Have a question? Having a technical issue?

Contact us in the U.S. at +1 727.733.2447 or info@oceanoptics.com



Our Application Scientists will assist you. For local contact details, see the inside front cover.



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