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May 2016 Volume 31 Number 5

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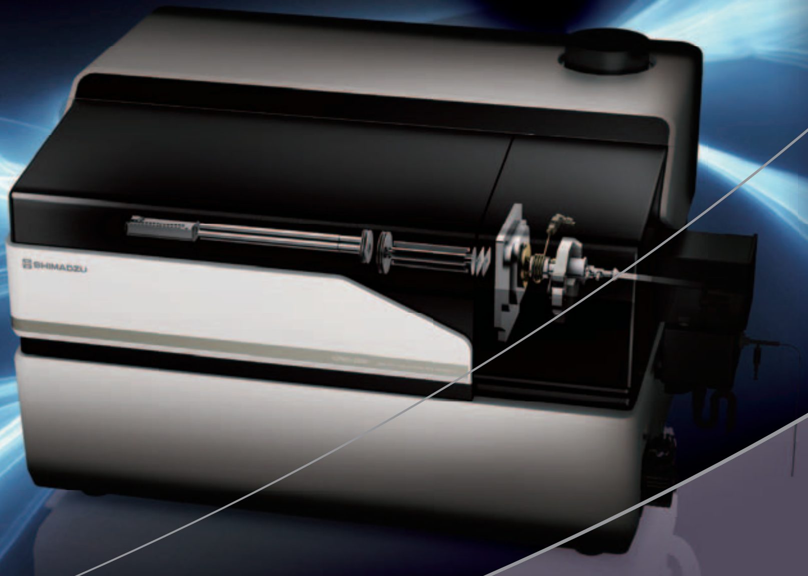

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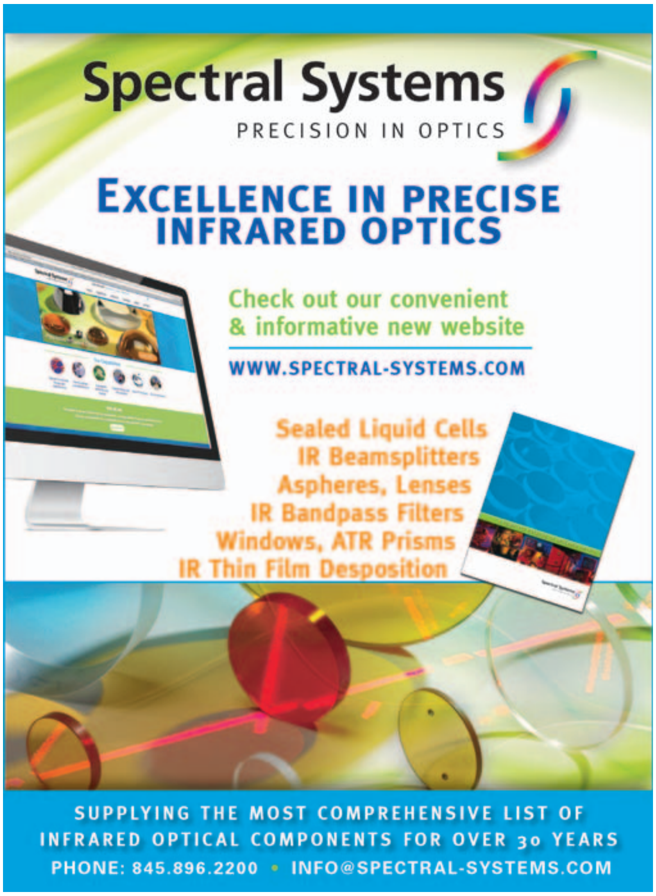

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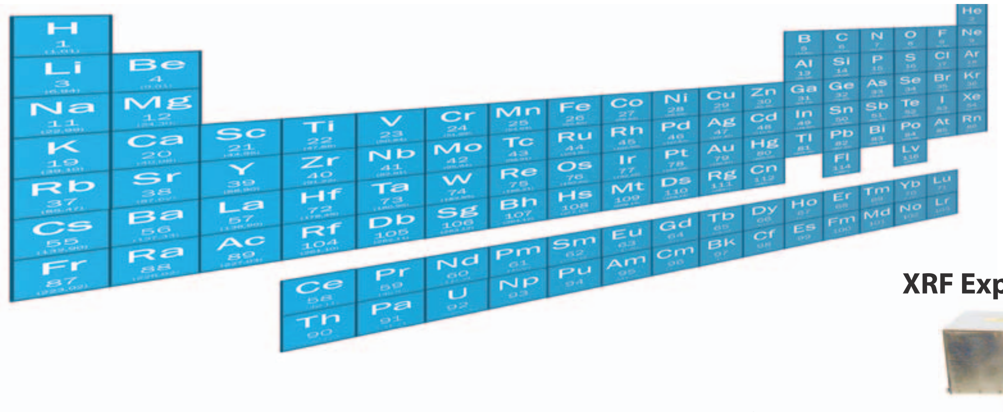

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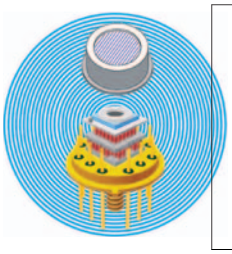

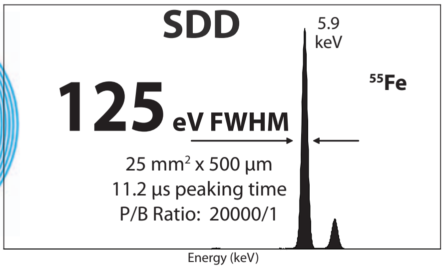

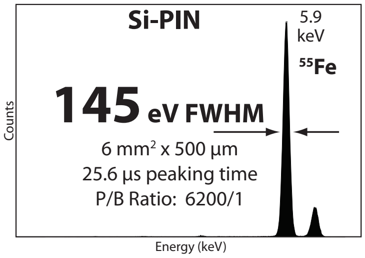

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ON THE WEB

QUIZ: INTERPRETING SPECTRA

Take the latest quiz!

Are your spectral interpretation skills up to par? Find out by taking the latest quiz from our "IR Spectral Interpretation Workshop" column.

See the quiz on page 38 of this issue or at:

spectroscopyonline.com/ ir-spectral-interpretation-workshop-o

WEB SEMINARS

Preparation and Elemental Analysis of Foodstuffs Using Microwave Assisted Sample Digestion and ICP-OES
Olaf Schulz, Spectro Analytical Instruments and Ulf Sengutta, CEM GmbH

***USP* 232 and 233: Understanding Method Requirements and Guidance for Getting Your Laboratory Ready for Implementation**
Johan Nortje, Milestone Inc., and Francine Walker, Chemical Solutions

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Maura Rury
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FEATURED ARTICLE

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Howard Mark and Mike Bradley
Our annual review of products—introduced at Pittcon or during the previous year—broken down into the following categories:

DEPARTMENTS

Spectroscopy (ISSN 0887-6703 [print], ISSN 1939-1900 [digital]) is published monthly by UBM Life Sciences 131 West First Street, Duluth, MN 55802-2065. Spectroscopy is distributed free of charge to users and specifiers of spectroscopic equipment in the United States. *Spectroscopy* is available on a paid subscription basis to nonqualified readers at the rate of: U.S. and possessions: 1 year (12 issues), $74.95; 2 years (24 issues), $134.50. Canada/Mexico: 1 year, $95; 2 years, $150. International: 1 year (12 issues), $140; 2 years (24 issues), $250. Periodicals postage paid at Duluth, MN 55806 and at additional mailing offices. POSTMASTER: Send address changes to Spectroscopy, P.O. Box 6196, Duluth, MN 55806-6196. PUBLICATIONS MAIL AGREEMENT NO. 40612608, Return Undeliverable Canadian Addresses to: IMEX Global Solutions, P. O. Box 25542, London, ON N6C 6B2, CANADA. Canadian GST number: R-124213133RT001. Printed in the U.S.A.

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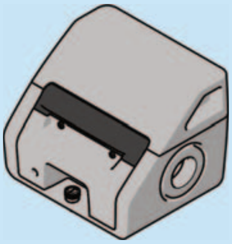
IRON LEVELS are often monitored in drinking water with spectroscopy, to meet EPA/EU guideline levels.

AN IMPURITY often found in diamonds using FTIR is nitrogen. It is thought to lend a yellow or brown colour to the stone.

hydrogen 1 H																	helium 2 He
lithium 3 Li	beryllium 4 Be											boron 5 B	carbon 6 C	nitrogen 7 N	oxygen 8 O	fluorine 9 F	neon 10 Ne
sodium 11 Na	magnesium 12 Mg											aluminium 13 Al	silicon 14 Si	phosphorus 15 P	sulphur 16 S	chlorine 17 Cl	argon 18 Ar
potassium 19 K	calcium 20 Ca	scandium 21 Sc	titanium 22 Ti	vanadium 23 V	chromium 24 Cr	manganese 25 Mn	Iron 26 Fe	cobalt 27 Co	nickel 28 Ni	copper 29 Cu	zinc 30 Zn	gallium 31 Ga	germanium 32 Ge	arsenic 33 As	selenium 34 Se	bromine 35 Br	krypton 36 Kr
rubidium 37 Rb	strontium 38 Sr	yttrium 39 Y	zirconium 40 Zr	niobium 41 Nb	molybdenum 42 Mo	technetium 43 Tc	ruthenium 44 Ru	rhodium 45 Rh	palladium 46 Pd	silver 47 Ag	cadmium 48 Cd	indium 49 In	tin 50 Sn	antimony 51 Sb	tellurium 52 Te	iodine 53 I	xenon 54 Xe
caesium 55 Cs	barium 56 Ba	57-71	hafnium 72 Hf	tantalum 73 Ta	tungsten 74 W	rhenium 75 Re	osmium 76 Os	iridium 77 Ir	platinum 78 Pt	gold 79 Au	mercury 80 Hg	thallium 81 Tl	lead 82 Pb	bismuth 83 Bi	polonium 84 Po	astatine 85 At	radon 86 Rn
francium 87 Fr	radium 88 Ra	89-103	rutherfordium 104 Rf	dubnium 105 Db	seaborgium 106 Sg	bohrium 107 Bh	hassium 108 Hs	meitnerium 109 Mt	darmstadtium 110 Ds	roentgenium 111 Rg	copernicium 112 Cn	ununtrium 113 Uut	flerovium 114 Fl	ununpentium 115 Uup	livermorium 116 Lv	ununseptium 117 Uus	ununoctium 118 Uuo

TUNA FISH are quickly tested for mercury with FTIR as they are moved through processing.

HEIGHTENED SEISMIC ACTIVITY (e.g. magma movement) can correlate with changes in ^{3}He/^{4}He levels in soil & water, detectable via spectroscopy.



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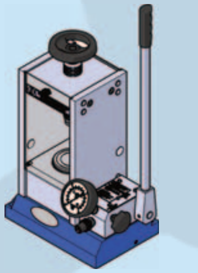

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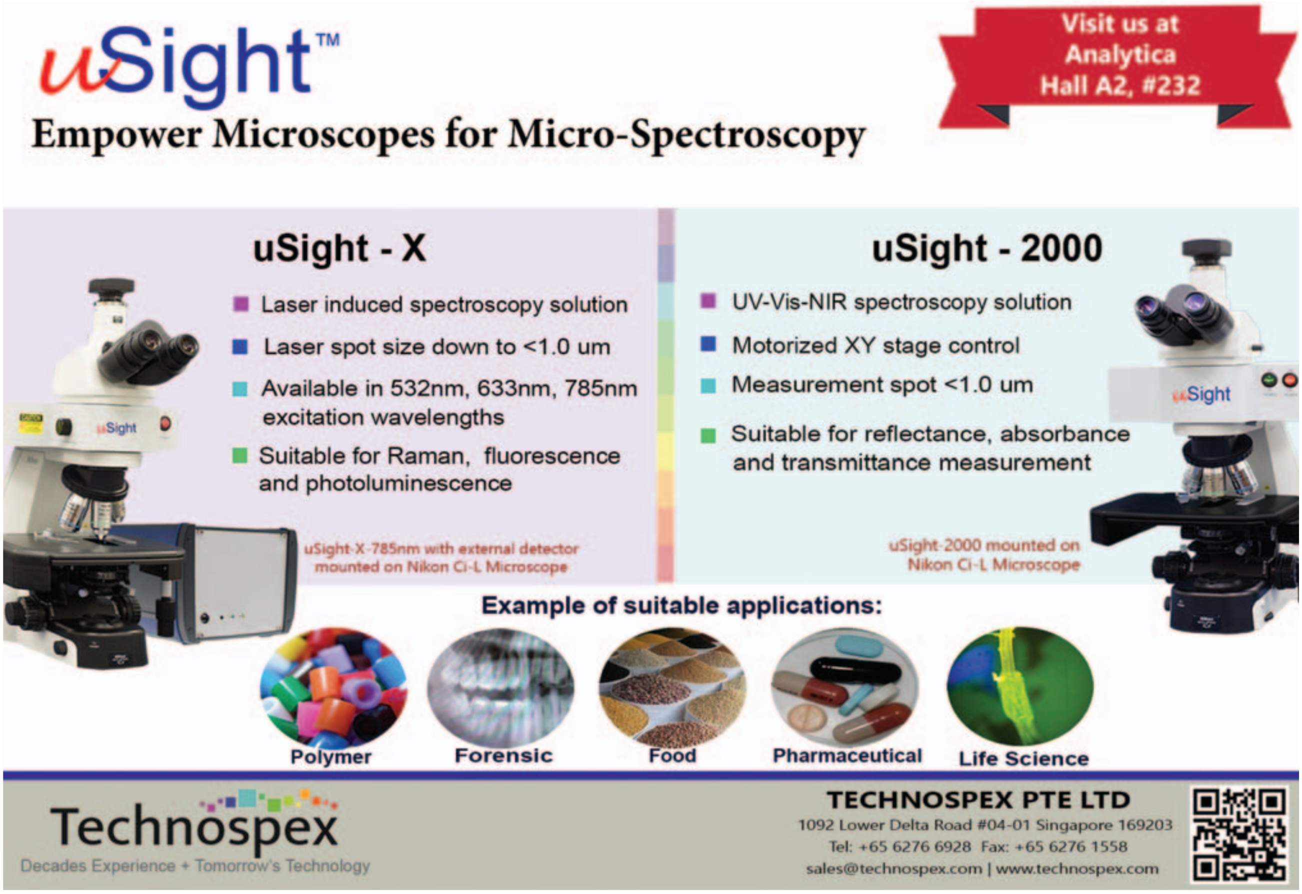

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News Spectrum

Bernhard Lendl Joins *Spectroscopy's* Editorial Advisory Board

Spectroscopy magazine is pleased to announce the addition of Bernhard Lendl to its editorial advisory board.

Lendl heads the research division on environmental and process analytical chemistry at the Technische Universität Wien (TUW) in Wien, Austria, where he was appointed full professor of vibrational spectroscopy in 2016. He received his PhD in technical chemistry from TUW in 1996, where he was a research assistant from 1994–2001. He worked as a guest professor at the Universidad de Córdoba, in Spain. In 2008, he founded the TUW spin-off company QuantaRed Technologies GmbH.

Lendl's research focuses on advancing analytical sciences through the development of novel analytical techniques and instrumentation based on infrared and Raman spectroscopy and their application to environmental and process analytical chemistry, material characterization, and biomedical diagnostics. His scientific work is documented in more than 200 papers published in international journals, 12 book chapters, and several patents. He received the Robert Kellner Lecture DAC (EuCheMS) in 2015, the FACSS Innovation Award in 2011, the Dr. Wolfgang Houska Award (B&C Foundation) in 2008, the Christian Doppler Award (government of Salzburg) in 2004, and the Fritz Pregl Award (Austrian Academy of Sciences) in 2002.

In July 2015, Lendl organized the 8th International Conference on Advanced Vibrational Spectroscopy (ICAVS-8) in Vienna, Austria, drawing 650 participants.

Jüergen Popp Wins Pittsburgh Spectroscopy Award

Jüergen Popp, a chair-holder of physical chemistry at the Friedrich-Schiller University Jena (Jena, Thuringia, Germany), was presented with the Pittsburgh Spectroscopy Award on March 8 at Pittcon 2016 in Atlanta, Georgia. He has served as the Scientific Director of the Leibniz Institute of Photonic Technology (Jena, Thuringia, Germany) since 2006.

Popp's research interests are in the areas of biophotonics and material sciences, in particular, the development and application of innovative Raman techniques for biomedical diagnostics as well as environmental and food analysis. He and his group focus on the development of noninvasive photonic microspectroscopic methods for in vitro and in vivo detection and characterization of heme and heme degradation products (HHDPs) and HHDP–peptide interactions.

Sanford A. Asher Wins Pittsburgh Analytical Chemistry Award

Sanford A. Asher, a Distinguished Professor of Chemistry at the University of Pittsburgh (Pittsburgh, Pennsylvania), was presented with the Pittsburgh Analytical Chemistry Award on March 8 at Pittcon 2016 in Atlanta, Georgia.

Asher pioneered the development of deep ultraviolet resonance spectroscopy for use in biophysical, physical, and analytical chemistry. His group developed both instrumentation and methodologies for determining protein structure and protein folding. Among the projects Asher and his group have in the works are the development of standoff instruments for the detection of explosive molecules, and the development of novel photonic crystal optical devices and responsive materials.

Asher received his PhD in chemistry from the University of California, Berkeley, and was a postdoctoral fellow at Harvard University (Cambridge, Massachusetts) in applied physics. He is the author of more than 290 publications and holds more than 29 patents in the area of photonic crystals. ■

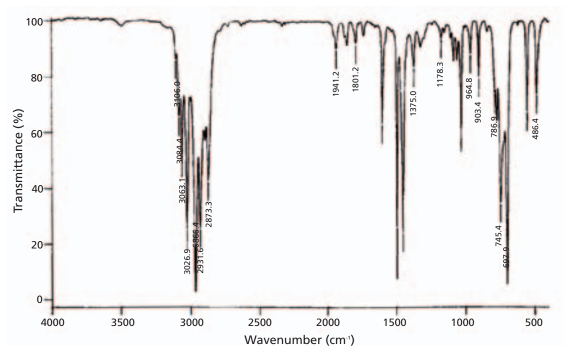
IR QUIZ TIME

Do your best to assign all the peaks shown in the figure and table to determine the functional groups present. There is one aspect of this molecule's structure you will not be able to determine, as we have not yet talked about it in the "IR Spectral Interpretation" column. The figure shows the IR spectrum of a liquid. Feel free to make use of reference spectra already published in the column.

To see the answer, please turn to page 38 in this issue.

Visit the link below to take this quiz (and others) online.

The peak positions for the problem spectrum		
3084	2931	1453
3063	2873	1375
3027	1604	745
2968	1495	697



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Method development for ICP-OES

Matthew Cassap, ICP-OES Product Manager, Thermo Fisher Scientific

To learn more about Method development for ICP-OES, Spectroscopy Magazine talked with Matthew Cassap, Product Manager ICP-OES and AA, at Thermo Fisher Scientific. After graduating in chemistry, Matthew worked at the British Standards Institute and later for the Centre for Environment, Fisheries and Aquaculture Science (a British government laboratory), supporting a number of National and European marine monitoring programs. In 2006 Matthew joined Thermo as an applications specialist becoming an expert in trace element analysis across a broad range of industry segments. In 2012 Matthew assumed responsibility for the Thermo ICP-OES product line in Cambridge, UK and since 2014 has been based at the Thermo Center of Excellence in Bremen, Germany as AA and ICP-OES Product Manager.

Spectroscopy Magazine: Can you provide a short description of ICP-OES and some of the typical applications?
Matthew Cassap: ICP-OES is a multi-element technique used for the identification and quantification of elements. A liquid sample is converted to an aerosol and transported to the plasma using a nebulizer and spray chamber ensuring only small droplets are transferred to the plasma. In the plasma the sample undergoes desolvation, vaporization, atomization and ionization. The atoms and ions then absorb energy from the plasma which causes electrons within them to move from one energy level to another. When the electrons fall back to ground state a photon of light is emitted at a specific energy or wavelength. The amount of light is directly proportional to the concentration of the element in the sample. Typical applications include the analysis of drinking, ground and sea water, quality control of products like alloys, and monitoring of food and supplements for nutritional elements.

Spectroscopy Magazine: What are the first steps in the process of developing a method for ICP-OES that should be considered?
Matthew Cassap: The initial selection of the sample introduction system such as the combination of nebulizer and spray chamber is critical and dependent on the sample type. The aerosol produced from the samples travels thru the spray chamber where large droplets are removed and smaller droplets are transported to the plasma. As the amount of dissolved solids in a sample increase (e.g. drinking water versus sea water) the tolerance of the plasma will decrease so a slightly less efficient sample introduction system is required. Once the correct sample introduction system is selected parameters including plasma settings and analysis wavelengths are selected. The plasma conditions depend on the matrix and the wavelength's to be measured; the combination of matrix and wavelengths are critical factors in setting the plasma power. The same is true with gas flows within the plasma.

Spectroscopy Magazine: For more advanced applications or matrices what different or additional steps would you take?
Matthew Cassap: An example of a more advanced application is the analysis of volatile organic samples. As the volatility of the sample increases much more of the sample is transported to the plasma causing instability and conversion of the organic solvent into an aerosol or gas. Since at room temperature and pressure one mole of a gas is 24L in volume, changing the solvent into a gas suddenly increases the flow into the plasma. To compensate for the extra volume the spray chamber is cooled to condense the gas back to a liquid for removal. In addition, when organic matrices are introduced, a high concentration of elements that emit light (e.g. carbon) not only at discreet wavelengths but also in large molecular emission bands across the spectrum can also be introduced, and these interferences have also to be taken into account when selecting method parameters.

Spectroscopy Magazine: Are there any steps that can be taken during the method development process to mitigate interferences?
Matthew Cassap: There are three main types of interferences in ICP-OES analyses: physical, chemical and spectral. Physical in-

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terferences are characterized as a difference between the samples and calibration standards affecting the sample transport or nebulization. These differences can be viscosity, density, and matrix differences, either from the sample itself or the digestion/preservation procedure and can usually be alleviated by dilution. Care must be taken not to dilute a sample below the analytical range of the instrument. Matrix-matching is the process of closely matching the constituents of the calibration solutions and the samples. Matrix-matching is an ideal solution to negate physical interference and is the preferred analysis technique for most applications. The method of standard addition is also an excellent way of negating matrix effects, as the sample acts as its own calibration matrix. The Thermo Scientific™ iCAP™ 7000 Plus Series ICP-OES software automatically calculates the sample concentration for standard addition methods. Where full matrix matching is not possible acid matching is generally accepted, although it is not a substitute for complete matrix-matching. Internal standard addition is also a popular method used to overcome sample transport effects. The internal standard (normally aspirated continuously via a Y-piece and mixing loop) acts as dynamic drift correction and Thermo Scientific™ iCAP™ 7000 Plus Series ICP-OES Qtegra ISDS automatically corrects either during or post-analysis for any enhancement or suppression of the sample response.

Chemical interferences can also occur due to differences between the sample and calibration standard reactions to ionization, molecular formation and plasma loading. Chemical interferences can be caused by ionization or molecular formation in the plasma and can either suppress or enhance a signal. Dilution, matrix matching and internal standardization, along with plasma optimization and sample doping can all be used to mitigate chemical interferences. Plasma optimization can also be used to vary the energy available in the plasma and also increase or decrease the sensitivity of specific wavelengths by altering the RF power, and the auxiliary and nebulizer gas flow. These adjustments are normally done during method development and often alleviate plasma loading and ionization problems simply by optimizing the method parameters. Ionization problems are common with samples that contain high concentrations of easily ionized elements (EIEs) such as sodium, potassium and calcium. These elements take energy from the plasma and can result in poor results for wavelengths below 235 nm which require high energy to reach excitation and an emission state. The use of an ionization buffer can often alleviate this problem; plasma optimization techniques also commonly involve doping the samples (normally by continuous aspiration via a Y-piece and mixing loop) with EIEs like cesium or lithium.

Spectral interferences are characterized by either partial or direct overlap of the analyte of interest by an interfering element. They are normally apparent during method development and can lead to suppression or enhancement of signals, and false-negative or positive results which ultimately degrade the accuracy and precision of the method. Spectral interferences are sometimes severe in ICP-OES due to the effectiveness of the plasma as an excitation source and the complexity of the emission spectrum of the elements and their ions. These interferences can be a shoulder on a peak, or a partial or full spectral overlap. It is a challenge to analytically correct for a full spectral interference, so a wavelength experiencing this uncommon phenomenon would be eliminated at the early stages of method development. Partial and peak overlaps are dealt with by either off-peak background correction or with the use of an experimentally derived mathematical correction, or the use of wavelengths that are free from interferences in the first place.

Spectroscopy Magazine: What other tools are available during the method development process?
Matthew Cassap: There are a number of plasma optimization software tools available within the Qtegra ISDS software. With Qtegra ISDS there is a plasma optimization tool that uses multi-variant optimization which has significant advantages over univariate optimization. This tool can be used to optimize the analysis of all elements in a method, or only for those required. For elements such as potassium and calcium, sensitivity is not usually an issue and they are normally not included in the optimization in favor of other more critical elements like lead or arsenic. For spectral interferences, the Element Finder plug-in for the Qtegra ISDS software is a method development tool that allows the selection of wavelengths that are free from spectral interferences taking into account the analytes present in the sample and the sample matrix. This tool uses the “full frame” of the sample (a full frame is an image of the entire sample spectrum within the wavelength range of the instrument) and intelligently selects the wavelengths that are suited to analysis of the elements selected, saving considerable time through automation.

Spectroscopy Magazine: Once developed what steps can be taken to ensure that the method is accurate and precise?
Matthew Cassap: The most important items to check are the linear range of the method from the detection limit to the top standard level. If there are interferences, the proposed USP elemental impurity chapters describes a lengthy spiking method. A faster approach is to analyze range-certified reference materials over the range concentrations to be analyzed, followed by further validation with the USP spiking method.

Spectroscopy Magazine: Does that complete method development or is it an ongoing process?
Matthew Cassap: Since the long term stability and robustness of the method is important it is an ongoing process. Methods need to ensure that detection limits are achievable over long periods of time, with different operators and a range of samples. Samples containing a different set of elements compared to the samples that were used for method development may require wavelengths to be revisited. Instrument maintenance should be written into SOPs forming an integral part of any method. The frequency of these checks should be refined as the method is used for daily analysis.

Atomic Perspectives

The Importance of Method Development for Trace-Element Analysis by Inductively Coupled Plasma–Optical Emission Spectroscopy

Selecting the correct wavelengths or isotopes and optimizing flame, furnace, or plasma conditions can seem like a daunting task for a novice user, with a multitude of opportunities to introduce errors and generate poor quality data. While most elemental analysis instruments have intuitive operating software, they lack the intelligence to guide operators through the early stages of method development and overcome associated problems along the way. This study describes an automated, intelligent approach to method development for trace-element analysis using optical emission spectroscopy, and exemplifies this capability with a suite of real-world sample matrices.

Maura Rury

Since its introduction more than 40 years ago, inductively coupled plasma–optical emission spectroscopy (ICP-OES) has significantly changed the capabilities of elemental analysis. This technique combined the energy of an argon-based plasma with an optical spectrometer and detection system capable of measuring low-level emission signals, which allowed laboratories to perform rapid, automated, multielement analyses at trace concentrations (1). This introduction occurred approximately 10 years before the introduction of the first commercial inductively coupled plasma–mass spectrometry (ICP-MS) system, so ICP-OES systems became the workhorse instruments in many laboratories required to perform elemental analysis at trace-level concentrations. The sensitivity, speed of analysis, ease of use, and tolerance to high levels of dissolved solids makes ICP-OES a technique that laboratories continue to rely on, decades after its inception (2,3).

As with many techniques, its success in the laboratory depends upon the quality of the methods that are developed for the application work being conducted. While ICP-OES instruments provide automated, intuitive operation with parts-per-billion detection limits and working ranges that extend over several orders of magnitude, developing a useful, well optimized analytical method can be a labor-intensive and time-consuming process.

The quality of any developed and optimized analytical method can be assessed by a number of different figures of merit, including accuracy, precision, sensitivity, speed, working range, ease-of-use, and reproducibility. Both the instrument operating conditions and method parameters can affect these performance characteristics, so it is important to be familiar with these factors and understand their effects on the analytical data being collected.

It is not the intention of this column installment to denigrate the importance of developing an optimum sample preparation method for a given sample type. If sample preparation is not approached with careful and thoughtful consideration, the instru-

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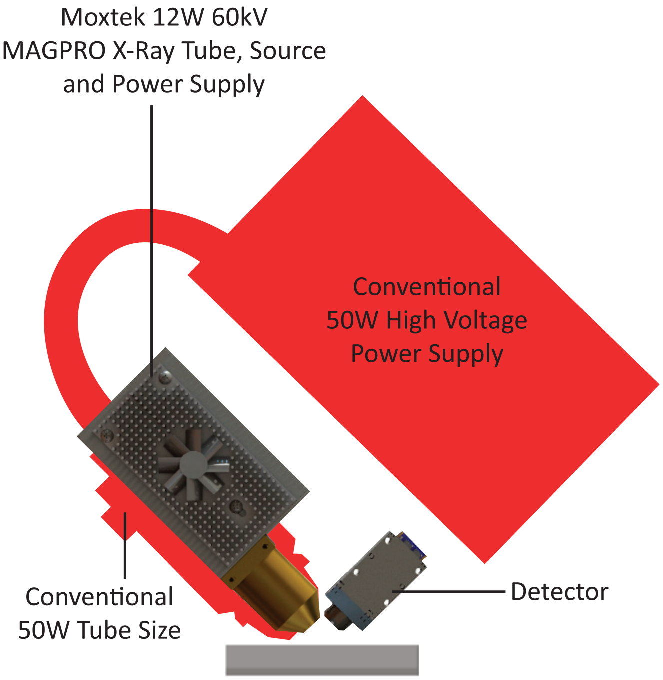

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ment method will not compensate for it. There are many potential pitfalls when preparing samples for analysis, including contamination, loss of volatile elements, incomplete dissolution, creation of an unstable solution, and alteration of the elemental species present in the original sample. Any of these issues will produce poor quality data, regardless of the robustness of the instrument method. However, for the purposes of this article, it will be assumed that optimized sample preparation procedures have been developed.

Method Development Considerations

Whether a method is being developed from scratch or an existing method is being further optimized, there are a number of parameters that should be taken into consideration to ensure the method is best suited for the intended application. These include

- Analytical wavelengths
- Interferences
- Plasma parameters
- Data acquisition parameters
- Validation of method

Let's take a look at each of these considerations, in turn, to understand how each factor plays a role in the quality of the final optimized method. It should be noted that the theory behind this approach is applicable to the development of an analytical method for any elemental analysis technique; however, some of the specific considerations will change. For example, if developing an analytical method for an ICP-MS application, one would be choosing isotopes instead of emission wavelengths for measuring the analytes and internal standards.

Analytical Wavelengths

When choosing appropriate wavelengths for the elements of interest, it's important to keep in mind the method's desired performance attributes. For example, if method development is taking place for quantifying trace elements in drinking water samples, the main performance attributes will likely be detection capability and accuracy. Therefore, the most sensitive wavelength should be chosen for each element and all potential interferences should be identified and carefully corrected. Alternatively, if a method is being developed to quantify elements in oil additives a wider working range may be desired. In this case, wavelengths with lower sensitivity may need to be chosen to maximize the concentration range over which the elements can be calibrated.

A critical factor in determining the suitability of a wavelength is whether it suffers from interferences. Several types of interferences exist in ICP-OES, and their severity is dependent on the analyte wavelength, other elements present in the sample, and the sample matrix itself (4). Evaluating interferences is not a trivial task and must be carried out with a great deal of care and thought. Interferences that are erroneously identified or not compensated for correctly will result in poor quality data. With the number of interference types and the variety of correction approaches possible, interference correction can quickly become an overwhelming task, particularly to an inexperienced operator. For this reason, when addressing interferences the following wavelength

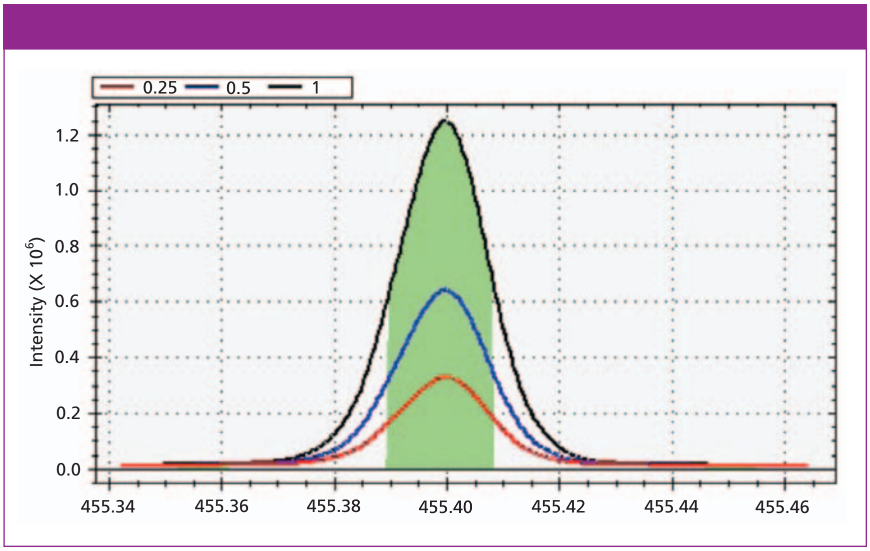


Figure 1: Examples of emission profiles for three calibration standards and a blank.

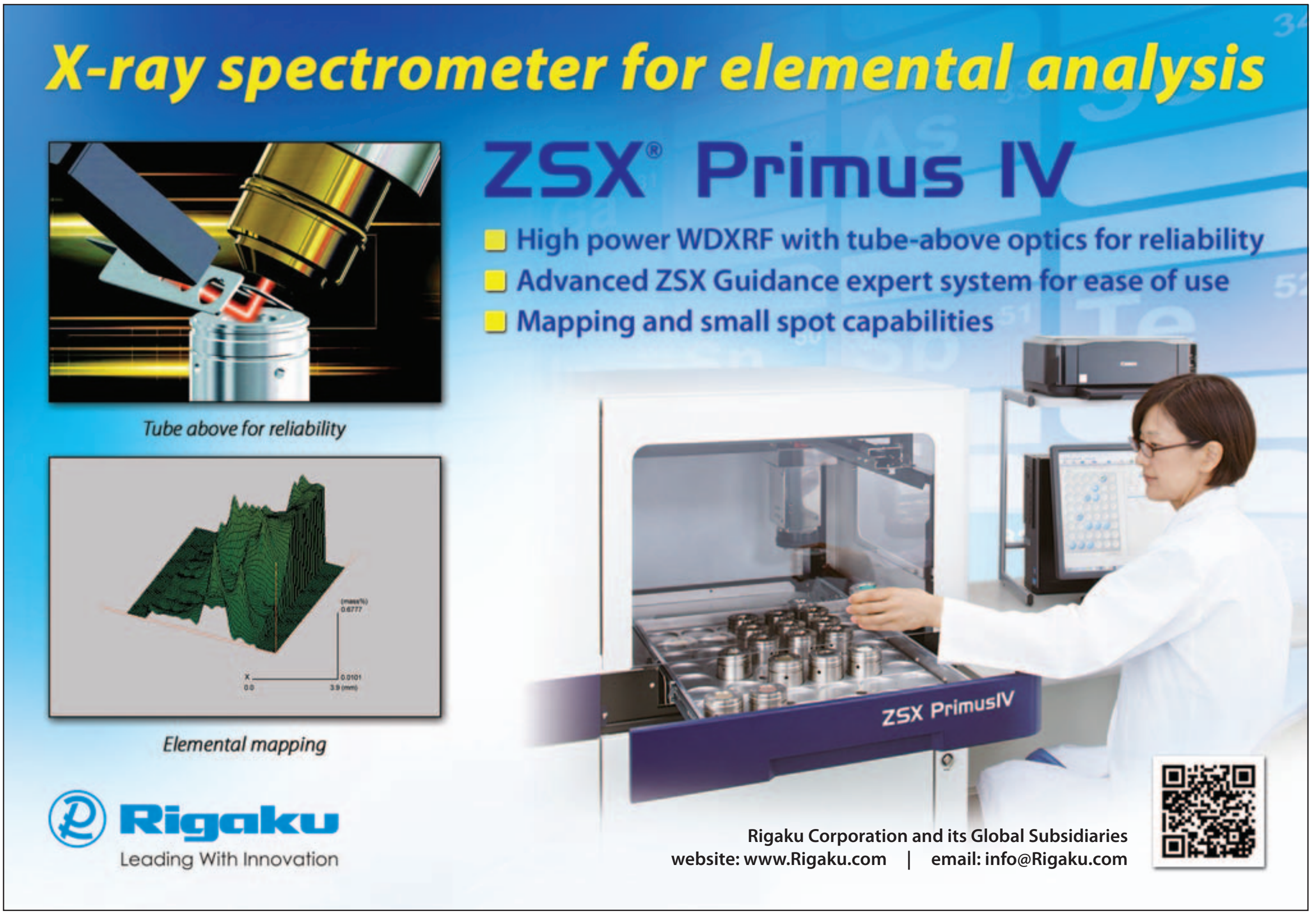
selection procedure is recommended:

1. Choose several wavelengths for each element in the method
2. Collect analyte wavelength scans
3. Visually inspect the peaks for the data collected
4. Review data
5. Eliminate unsuitable wavelengths

Let's review this process in more detail. In the first step, it is recommended to choose two or three wavelengths for each element of interest. This includes both the analyte elements and any applicable internal standard elements. Typically, the most sensitive wavelength for each element would be chosen, along with two wavelengths of slightly lower sensitivity. If a wide range of concentrations is expected to be encountered in the samples, a high sensitivity wavelength might be chosen along with a low sensitivity wavelength. In some cases, the sample matrix will produce an emission spectrum that is so complex, there may be only one or two suitable wavelengths (interference free and providing the desired working concentration range) to choose for the analysis.

After a set of wavelengths has been chosen for evaluation, data should be collected to determine which wavelengths are best suited, based on the requirements of the application. It is recommended that three wavelength measurements be collected for each of the following solutions:

- A blank (calibration and method blanks, where applicable)
- A low-concentration calibration standard
- A high-concentration calibration standard
- A sample that represents each type of sample matrix to be analyzed



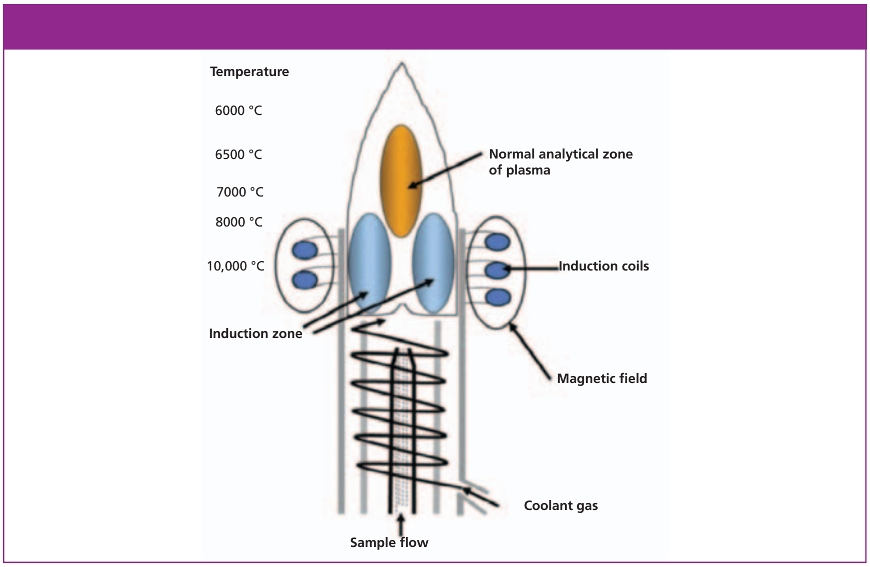


Figure 2: Different temperature zones within a plasma discharge.

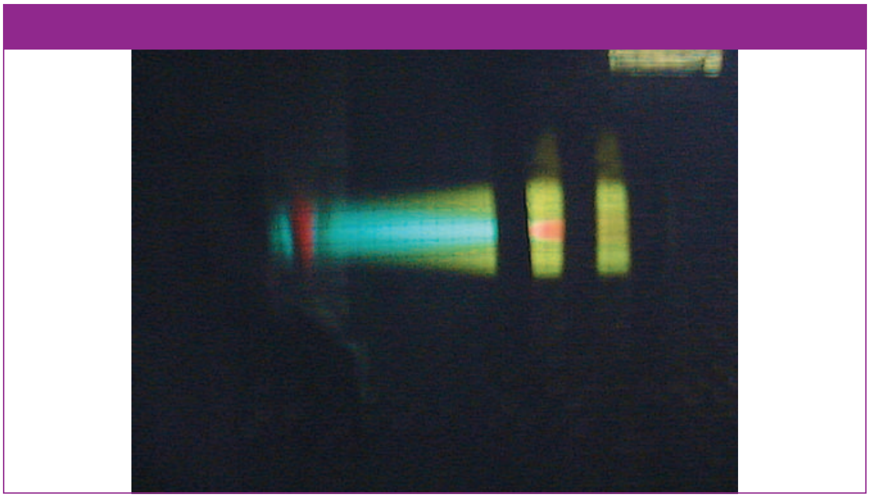


Figure 3: An example of how the plasma tail is removed.

Data from the blank provides an emission profile of the matrix in the absence of analytes. Data from the calibration standards provides profiles for the elements of interest at low and high concentrations. Both sets of measurements are required for the data inspection outlined in steps 3 and 4 described earlier. The highest concentration calibration standard should be used for this data collection to ensure that none of the selected wavelengths suffer from peak broadening or self-absorption (5). Sample measurements produce emission profiles for the elements of interest in the presence of the sample matrix. One sample for each matrix type should be collected to ensure emission profiles are examined in every applicable sample matrix. For laboratories analyzing a wide range of sample matrices, collecting wavelength measurement scans for each matrix type could require data collection for a large number of samples.

After wavelength data has been collected, they should be visually inspected to determine that the emission peaks have the proper shape and size. An ideal wavelength would produce the series of emission signals illustrated in Figure 1. In Figure 1, the emission from the blank produces a flat emission signal with a relatively low intensity. The emission signals for the calibration standards and representative samples should produce a symmetric, Gaussian-like shape with a single peak. Each peak should exhibit a proportional change in magnitude to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match the difference in concentrations. For example, data from a standard containing elements at 1.0 ppm would be expected to have approximately twice the signal of that for a 0.5 ppm standard, while maintaining approximately the same shape.

Numerical data should be inspected to determine the intensity and precision at each wavelength. The intensity for each standard should increase at a rate that is proportional to the increase in its concentration. If a set of three wavelength measurements was collected for each solution, the measured intensities can be used to calculate the approximate precision for each measured standard. Calculated precision values should be within the acceptable limits for the application.

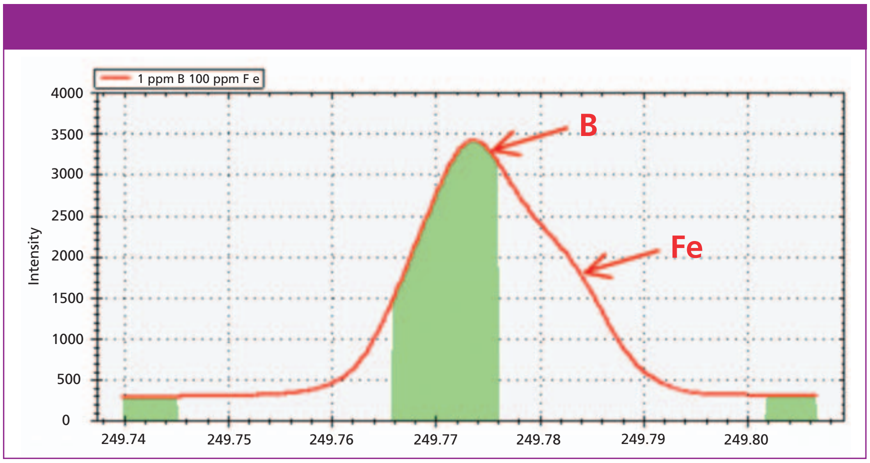


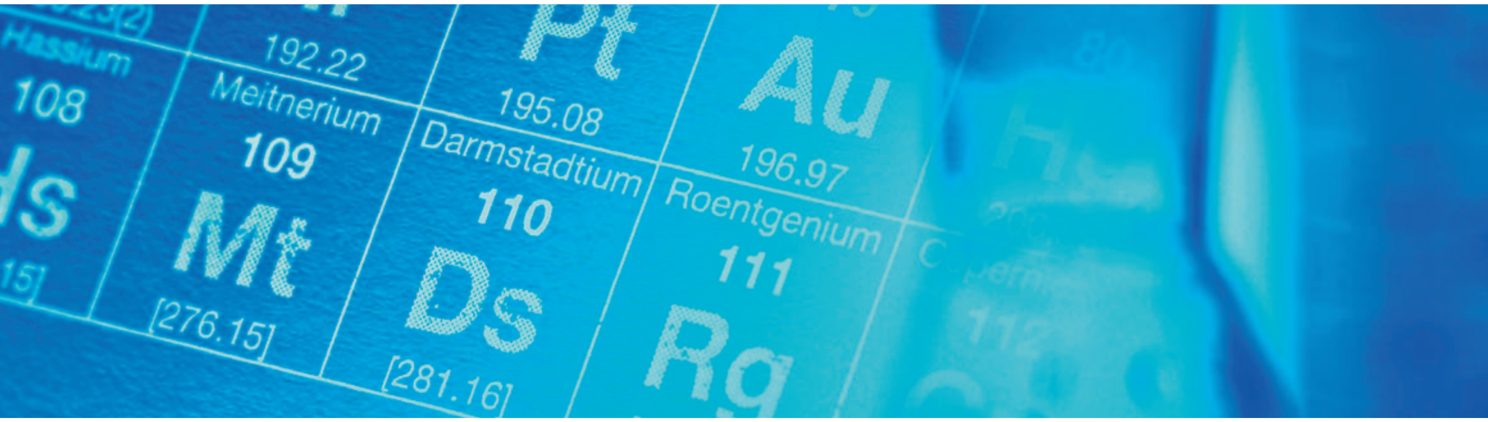
Figure 4: Emission profile of 1 ppm B in a matrix containing 100 ppm Fe.

Interferences

Interferences are common with any plasma-based technique, particularly when trying to measure trace-level concentrations in a sample matrix that contains high concentrations of elements that produce line-rich spectra, such as Fe, Ca, and Si (6). Sample matrices that are known to generate these types of interferences include geological, metallurgical, and high-matrix environmental samples, such as soils or wastewaters. The three common types of interferences in ICP-OES are physical, chemical and spectral.

Physical Interferences

Physical interferences occur when the nebulization or transport efficiency of the standards differs from that of the samples. These differences in the physical characteristics of the matrices (density, viscosity, level of dissolved solids) can produce errors in the measured sample concentrations. Physical interferences are typically not wavelength



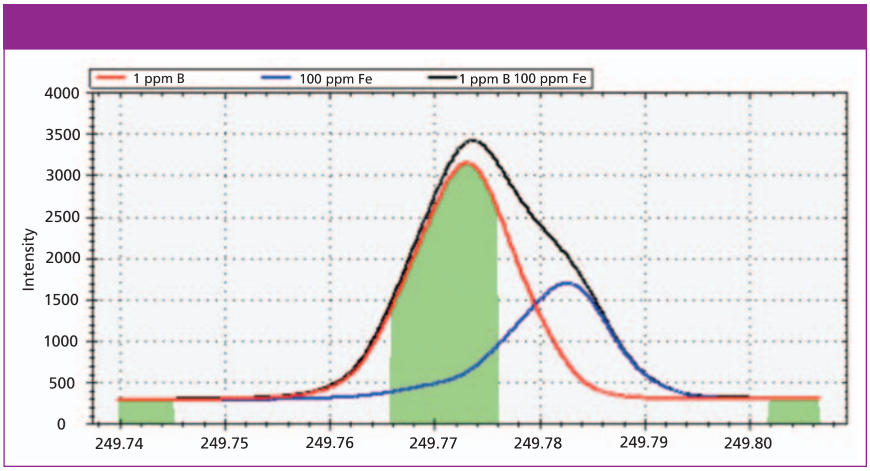


Figure 5: Emission profiles to demonstrate spectral overlap.

specific and can be overcome by using internal standards and preparing the calibration standards in a matrix that matches that of the samples (7).

Chemical Interferences

Chemical interferences occur when the standards behave differently from the samples as they enter the plasma. These types of interferences typically result from changes in temperature within the plasma and include easily ionized element (EIE) effects, molecular emission, and plasma loading. Referring to Figure 2 (4), the plasma consists of several temperature zones, which translate to varying amounts of energy available for excitation of the ground-state atoms. The plasma is hottest and contains the greatest amount of energy at its base, which is where the sample is introduced. In this region, the plasma contains sufficient energy to atomize and ionize elements before they are excited. Ionization is particularly prevalent for elements in the first two groups of the periodic table, which all have relatively low first ionization potentials. These easily ionized elements include elements such as Na, K, and Li.

When easily ionized elements are present at low concentrations, very few of the atoms become ionized, which means emission will take place from excited atoms. At high concentrations, a significant number of the atoms will become ionized, which shifts the emission wavelength such that it will predominantly occur from the excited ions. If left uncorrected, this interference will reduce the linear dynamic range of the calibration curve and can potentially produce highly inaccurate results (8).

This type of interference can be corrected by adding an ionization suppressant (also known as an ionization buffer) to all the solutions before analysis.

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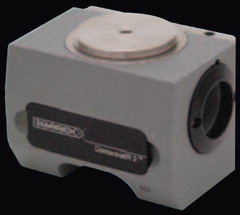

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An *ionization suppressant* is a solution containing a high concentration of an easily ionized element (1000 ppm Cs, for example). The solution will produce an extremely high concentration of cesium ions in the plasma, which, according to Le Châtelier's principle (9), will reduce the concentration of ions and increase the concentration of atoms to provide a chemical equilibrium balance in the plasma. Therefore, the element of interest will remain in its atomic state in the plasma.

If a dual-view instrument is being used, an additional step to take in correcting for this type of interference is to also measure the emission radially. EIE effects are much more significant for axial plasmas as emission is being measured from species that are present in all temperature zones within the central channel of the plasma. If emission is measured perpendicular to the direction of the plasma (radial view), emission will be measured from a single temperature zone (10).

Converse to the formation of EIE interferences are the formation of molecular interferences. If we refer again to Figure 2, the tip (also known as the tail) of the plasma is the coolest and least energetic part of the plasma (11). In this region, atoms and ions that were formed in the hotter part of the plasma can combine to form molecules. These molecules can become excited and emit light, which will produce broadband, molecular emission spectra.

This type of interference is relatively straightforward to correct and requires very little intervention from the analyst. Since the coolest part of the plasma is in its tail, removing that portion of the plasma prevents atoms and ions from traveling through a zone that's cool enough to allow them to combine and form molecular species. All modern ICP-OES instruments are set up to automatically and effectively remove the tail of the plasma. There are a variety of methods in which this is accomplished—a flow of inert gas that is counter to the direction of the plasma, a high velocity shear gas, or a cooled cone interface; however, all are effective in cutting off the tail of the plasma. An example of how the plasma tail is removed is illustrated in Figure 3.

As with chemical interferences, another option for eliminating molecular interferences is to measure emission from a radially configured plasma. If emission is collected at 90° to the plasma and the observation height is optimized, emission should be collected from the "normal analytical zone," which is well-separated from the cooler tail of the plasma.

Plasma loading is an interference that is sometimes experienced when samples contain organic solvents or high levels of dissolved solids (12). When a significant amount of material is introduced into the plasma, it cools the plasma and, in severe cases, can extinguish it completely. Cooling the plasma reduces the amount of available energy, which affects the emission intensity of the elements present. As a result, if samples contain concentrations of dissolved solids that are different from those in the standards, the emission intensity for the same analyte concentration will be different in the samples and standards which could produce data inaccuracies. This interference can usually be addressed by preparing standards in a matrix that matches that of the samples, using correct internal standards, choosing sample introduction components that were designed for the application, and selecting sample introduction conditions that minimize plasma loading.

Spectral Interferences

The third and sometimes most challenging type of interferences are spectral. These interferences occur when emission from one or more species in the sample matrix overlaps with the emission for the analyte of interest. These interferences can result in a background shift, a partial peak overlap, or a direct overlap. If the analyte is suffering from a direct spectral overlap, the interfering element must either be removed from all solutions before analysis, or an alternative wavelength must be selected. If the interfering element produces a simple background shift (either a flat, raised

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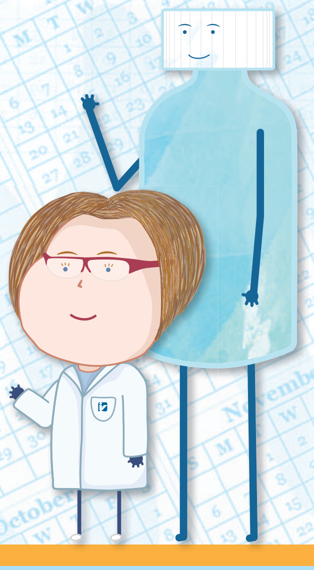

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baseline or a sloping background), the analyte can be accurately quantified by the use of optimized background correction points.

If the analyte suffers from partial spectral overlap, a combination of background correction and mathematical correction may need to be used. An example of partial spectral overlap is illustrated in Figure 4, which depicts data for a solution containing 1 ppm B in a matrix containing 100 ppm Fe.

A shoulder is clearly visible on the right side of the main peak, indicating the presence of a spectral overlap on B at 249.773 nm. If the emission profile for the sample solution is overlaid with that of single-element solutions containing 1 ppm B and 100 ppm Fe, the image in Figure 5 is produced.

In this figure, the red peak represents the emission profile for 1 ppm B at 249.773 nm, whereas the blue trace represents the emission peak for 100 ppm Fe at 249.782 nm. The black outline represents the combined emission from a sample containing 1 ppm B and 100 ppm Fe. The center green-shaded region represents the area under the peak that will be used for data collection. This area includes a portion of the emission peak from Fe and, if left uncorrected, this analytical measurement might produce erroneous data.

The best way to correct for this interference is to select an alternative emission wavelength for B that is free from interferences. If an alternative wavelength cannot be used, an interelement correction (IEC) factor should be calculated to correct for the overlap of Fe on B. If IEC factors are used, they must be carefully calculated and applied to ensure spectral overlaps are being accurately corrected. Improperly calculated IEC factors can produce data that are more erroneous than if no IEC factors were used (13).

Plasma Parameters

Optimum plasma operating conditions are as critical as correct wavelength selection and interference correction procedures. Plasma parameters will impact the stability and energy of the plasma and, therefore, the behavior of the elements, and are typically optimized to maximize the emission intensity for the analyte wavelengths in the method.

Plasma parameters to consider for optimization are

- RF power
- Nebulizer gas flow
- Auxiliary gas flow
- Coolant gas flow
- Radial viewing height

It should be noted that, while important, plasma optimization is usually not as critical as the other method development steps. ICP-OES methods typically are developed for the analysis of multiple elements. Each element prefers a slightly different set of plasma parameters to achieve its maximum intensity for the wavelength selected. Because ICP-OES instruments collect emission intensities from groups of elements simultaneously, it is not practical to select different plasma settings for each individual element. Therefore, the plasma settings for multielement analysis will be somewhat of a compromise for most of the elements in the method. Most modern ICP-OES instrumentation provides an automated optimization feature to rapidly and automatically select the best plasma parameters to maximize the emission intensity for as many elements as is possible in a multielement method (14).

Data Acquisition Parameters

The data acquisition parameters are another set of method development conditions to consider for optimization. They include the choice of axial or radial plasma viewing (if using a dual view instrument), the integration time, and the number of integrations. In general, an axial plasma is used for determining low, parts-per-billion concentrations, while a radial plasma view is used for higher (parts-per-million) concentrations or to help compensate for chemical interferences (15). The integration time for each plasma viewing configuration must be long enough to collect sufficient emission from all elements being measured. This time would usually be dictated by the element with the weakest emission line or the element that is present at the lowest concentration. An axial integration time of 15 s and a radial integration time of 5 s are fairly typical to use. Finally, the number of integrations or measurements must be set. Keep in mind that if every sample is collected using a single integration, statistical analysis and precision data and limits of quantitation cannot be calculated and reported. Therefore, two or more integrations must be collected for each sample to report this kind of information.

Validation

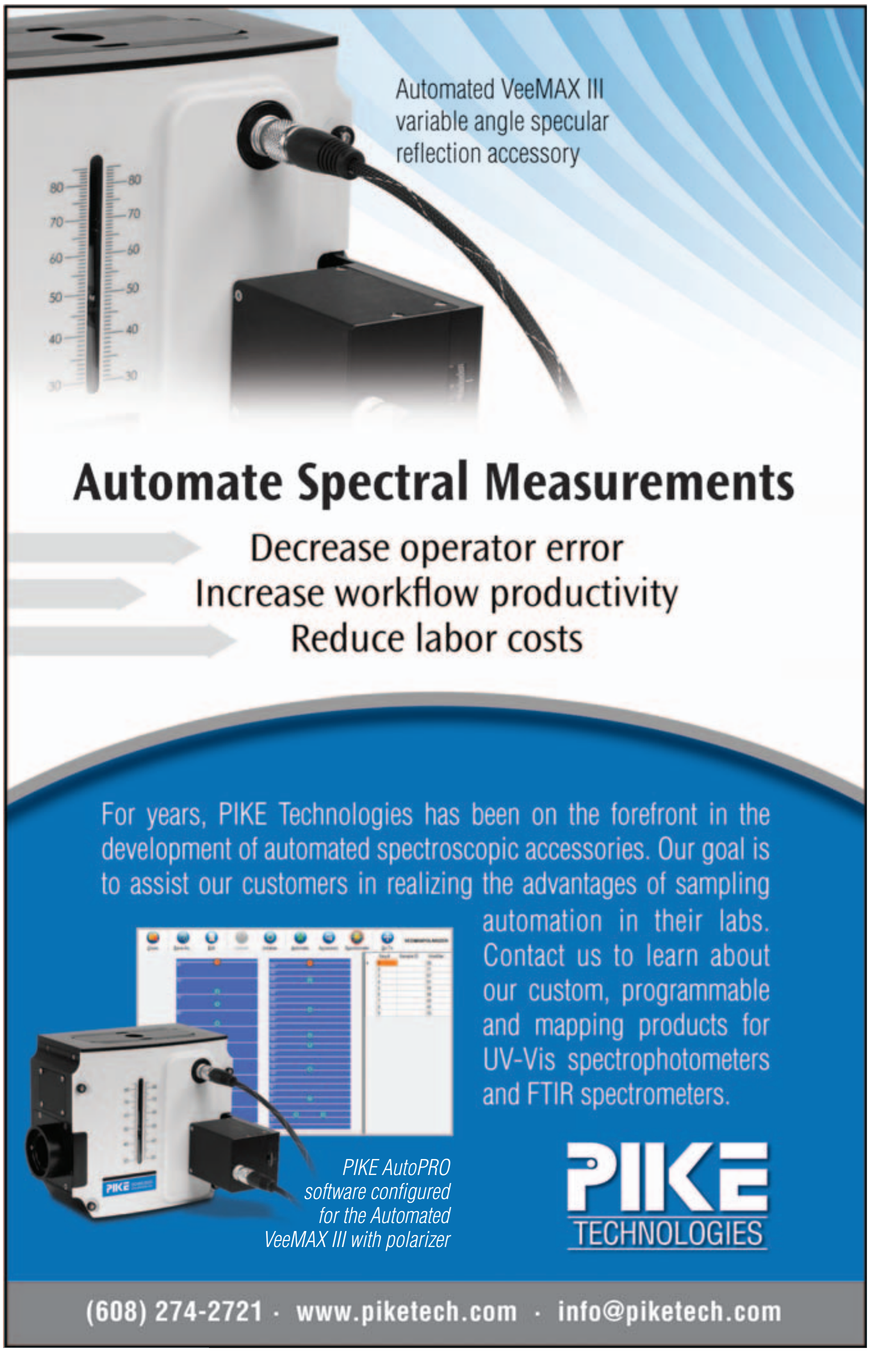
The final step in the method development process is to validate that the method will produce results that meet the figures of merit required for the application. Methodology that achieves good detection limits, yet cannot obtain the required accuracy is unlikely to meet the data quality objectives of the analysis. A detection limit study is always encouraged for any analytical method. Calculated detection limits and limits of quantitation allow reporting limits to be calculated to determine the lowest concentrations that can be measured and reported for a suite of elements in a given sample matrix (16).

Regardless of whether a detection limit study is performed, the developed method needs to be validated before use with real samples. The best approach to validating an analytical method is to obtain a certified reference material (CRM) that is appropriate for the application. If an analytical method is valid for the application, data acquired for a suitable CRM should match the certified concentrations that accompany the CRM (within defined error limits).

If a suitable CRM is not available for a given application, a number of other check standards can be used. A calibration standard can be prepared and analyzed as a sample to see if the concentration is at the level it should be. A calibration or quality control (QC) standard can be purchased from an external source and analyzed as a sample. Samples can be prepared and measured in duplicate to determine the precision of the method. Samples can be spiked with a known concentration of the elements of interest to determine whether the spiked elements can be measured and recovered at their expected concentrations. If interference corrections are being used, interference check standards can also be prepared or purchased and analyzed to ensure that the correct results are obtained.

Summary

Correct and optimized method development cannot be overemphasized when performing trace-element measurements by ICP-OES, or any other elemental analysis technique. Even though it can be a labor-intensive process, a poorly developed method has the potential to produce erroneous data. Conversely, a thoughtful method development strategy could be useful for several different applications with minimal modifications. This article



has provided an overview of some of the main factors that should be taken into consideration when developing an optimized ICP-OES method.

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For more information on this topic, please visit our homepage at: www.spectroscopyonline.com

SPECTROSCOPY SPOTLIGHT

Ensuring Product Quality with Process Raman and FT-IR Spectroscopy

John Wasylyk, a principal scientist at Bristol-Myers Squibb in New Brunswick, New Jersey, has been using quality by design (QbD), Raman spectroscopy, and Fourier transform infrared (FT-IR) spectroscopy in process development as well as for at-line and on-line monitoring of active pharmaceutical ingredient (API) crystallization. Here, he discusses the advantages, limitations, and challenges of these techniques.

How does your work with Raman spectroscopy fit into your company's approach to quality by design?

We have embraced the advantages of quality by design (QbD) and Raman spectroscopy and have reaped the benefits in terms of process knowledge, process optimization, and control. Raman plays an integral part of process development, as we have three platforms for implementation: walk-up (open access) instruments, portable laboratory instruments equipped with noncontact optics and probes for in situ data collection, and plant-based instruments. We have standardized on one laser type and manufacturer of Raman spectrometers, which enables us to transfer methods across all three platforms.

To promote QbD and the use of Raman spectroscopy to leverage our learning, we have held a series of training sessions hosted by both internal and external subject-matter experts covering topics from the basics of spectroscopy and instrument setup to more advanced principles of spectroscopy and in-line analytics. Furthermore, Raman has been key due to the ease of transferability across instruments and the availability of instruments that meet safety requirements in the US and Europe.

What are the advantages of coupling QbD with Raman spectroscopy in terms of understanding reaction kinetics and following the progression from development to manufacturing?

Regardless of the length of the time to run a reaction to completion, we can leave the Raman spectrometer in a programmable collection mode and use a variety of probes to cover the various sizes of reactors and sensitivity over a wide spectral range, all of which allow us to attain a complete kinetics profile for the reaction. Continuous data collection during QbD experiments allows us to capture the impact of parameter changes. In addition, this can include data collected during the scale-up process as well as the impact of physical-mechanical changes such as agitation rate, impeller variations, and heating and cooling rates. By using Raman spectroscopy throughout the entire development process we can obtain a broad understanding of critical reaction parameters that not only improves our speed to patients but also positively impacts the quality of our product.

> ***By using Raman spectroscopy throughout the entire development process we can obtain a broad understanding of critical reaction parameters that not only improves our speed to patients but also positively impacts the quality of our product.***

Your group has also used FT-IR spectroscopy to examine foreign materials in pharmaceutical development. What types of foreign materials were found, and how was FT-IR used to determine the source of the extraneous materials?

According to the Food and Drug Administration's (FDA) *Q7A Good Manufacturing Practice Guidance for Active Pharmaceutical Ingredients*, we are responsible for overseeing the quality of the incoming raw materials and intermediates. If a foreign material is found in an incoming material it will lead to an investigation and may ultimately lead to the rejection of that lot. Extraneous material can range from fragments of packaging material to process equipment components such as fragments of seals or gaskets. FT-IR allows for rapid classification and, many times, identification of extraneous material. We use commercial spectral libraries for the rapid classification and identification of foreign materials.

You have been using the mid-frequency and low-frequency spectral regions of Raman spectroscopy to study the transformation of amorphous indomethacin to the g-crystalline form (1). What are some of the challenges you faced in using this technique for this research?

Low-frequency Raman spectroscopy has been around for years, and one of

TOM FULLUM/GETTY IMAGES

the challenges was the lack of commercial Raman instruments that were capable of filtering out or attenuating the Rayleigh line to the point where low-frequency spectral bands could be observed. Recent advances in filters and gratings have affordably solved this challenge. Notably, this information may include the presence or absence of amorphous material in the crystalline matrix. In addition, the increased signal intensity in the low frequency range has allowed us, in a number of cases, to identify multiple polymorphs in the crystalline matrix. Coupling low- and mid-frequency (fingerprint) ranges has led to a wealth of information on both the short- and long-range crystalline structures. The recent addition of probes to the low-frequency-enabled instruments will help drive QbD during crystallization studies. The ultimate goal will be the advent of plant-based spectrometers that have both low- and mid-range capabilities.

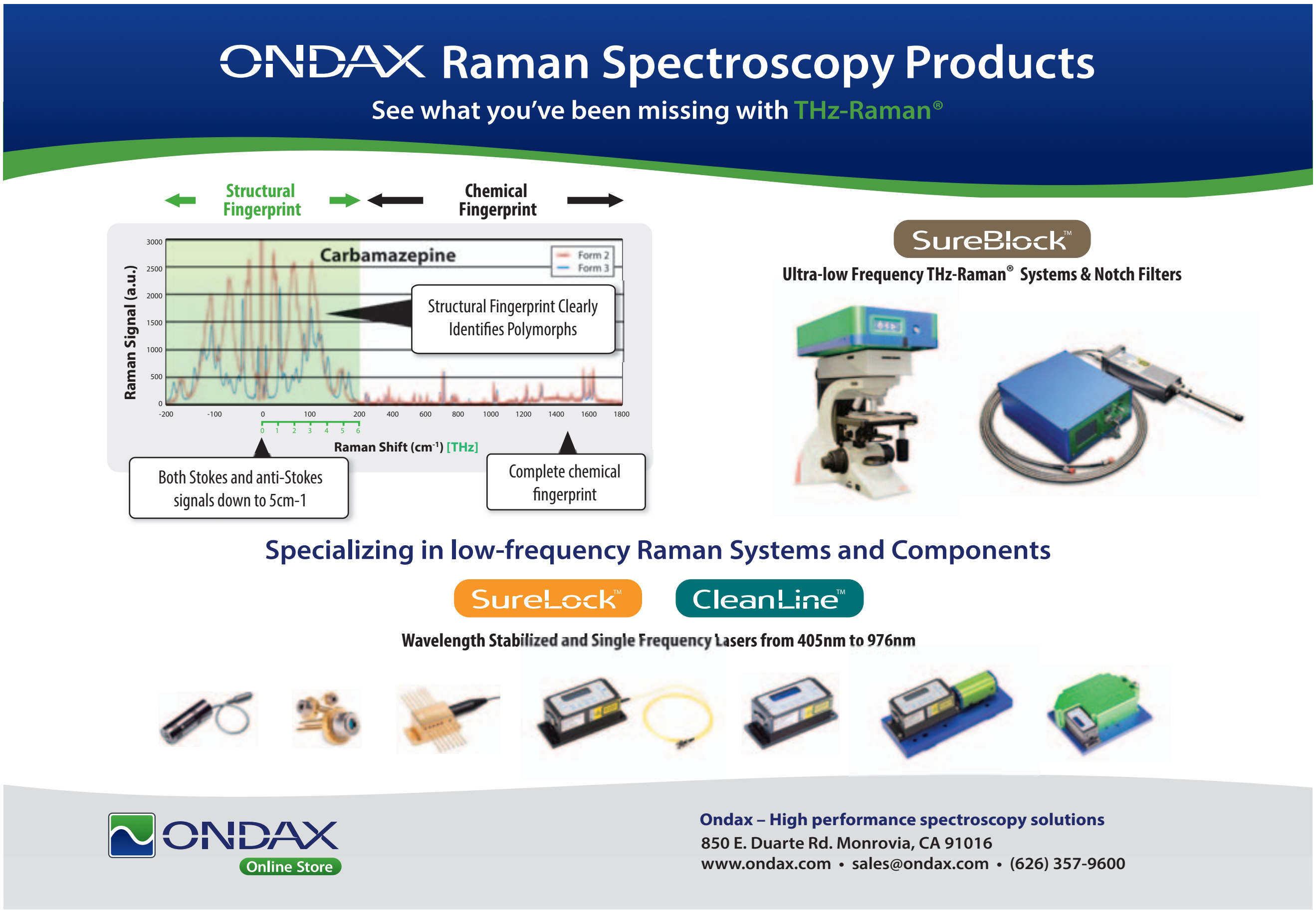
The Raman signal can travel long distances (we have fiber runs on the order of 75 m), enabling remote analysis of processes. This remote analysis capability means that we can follow a reaction or plant process in a rated or hazardous area and locate the actual spectrometer in a safe, nonhazardous zone.

What are the advantages of Raman spectroscopy for at-line and on-line monitoring of API crystallization?

There are several points I want to make here. First, manufacturers have developed lasers that are stable, reliable, and, from our experience, have an exceptionally long lifetime. This long lifetime is an advantage over other techniques such as FT-near infrared (NIR), which can require periodic changes of the light source. Second, instrument-to-instrument variability from the same manufacturer is minimal. The last point is that the Raman signal can travel long distances (we have fiber runs on the order of 75 m), enabling remote analysis of processes. This remote analysis capability means that we can follow a reaction or plant process in a rated or hazardous area and locate the actual spectrometer in a safe, nonhazardous zone. This is opposed to FT-IR and FT-NIR, which are limited to fiber bundles and can have a maximum fiber length for the transfer of spectral data of approximately 3 m.

Are there limitations or disadvantages to using Raman spectroscopy for that purpose?

A universal challenge when applying



Raman is the inherent fluorescence of the sample. Fluorescence, if intense enough, can saturate the detector (charge-coupled device [CCD] camera) and is more pronounced at lower laser wavelengths (532 nm > 785 nm > 1064 nm). However, one must balance the need for sensitivity with the desire to minimize the sample fluorescence. For instance, if I go to a higher wavelength laser, say, 1064 nm, it will minimize the sample fluorescence but it will also decrease the spectral band intensity, which may not be suitable to follow dilute reactions. Therefore, in certain cases, if the sample fluorescence cannot be mitigated, FT-IR, NIR, or UV may be the appropriate technique to choose.

What are the next steps in your research?

The next challenge that we are looking to tackle is to extend our application of Raman spectroscopy into the biopharma arena focusing on biologics both in processing streams to develop in-process controls, and in final isolated drug substance and formulations to develop release and quality control methods.

Reference

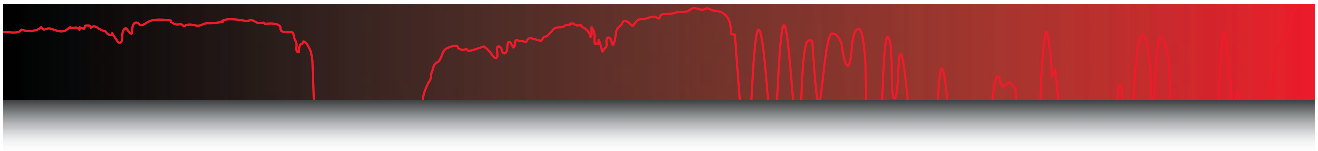
(1) P.J. Larkin, J. Wasylyk, and M. Raglione, *Appl. Spectrosc.* **69**(11), 1217–1228 (2015).

John Wasylyk is a principal scientist at Bristol-Myers Squibb in New Brunswick, New Jersey. For 25 years, he has worked with Chemical Development Operations and the Analytical and Bio-Analytical Department where he focuses on developing spectroscopy-based PAT methods for early- to late-stage development projects through to manufacturing, along with spectroscopy methods for reagents and foreign material investigations. He received his PhD from the State University of New York at Binghamton in Biology and an MS in Medicinal Chemistry from the University of Houston.

To read more recent interviews on various spectroscopy topics, please visit the "Interview of the Month" section on our homepage: spectroscopyonline.com.

Recent topics covered include:

- *Spectroscopy at the Interface*
- *Addressing the Challenges of Process Raman Spectroscopy*
- *Novel Optical Spectroscopy Techniques for Analyzing Nanoscale Structures*
- *How Are ICP Methods Being Used in the Petroleum and Biofuels Industry?*
- *Using SERS to Study How Cells Respond to Pharmaceuticals*
- *Tracking Biomolecules and Nanoparticle Probes in Biological Samples with Improved Microscopy Imaging Methods*
- *From Pharmaceutical to Agricultural Applications: What's New in NIR?*
- *Detecting Adulterated Meat with LIBS*
- *Diagnosing Disease with Raman Spectroscopy*
- *Miniaturized Quantum Cascade Lasers Enable Fast Mid-IR Spectroscopy* ■



IR Spectral Interpretation Workshop

Distinguishing Structural Isomers: Mono- and Disubstituted Benzene Rings

Following up on the last installment, we examine the infrared (IR) spectra of mono- and disubstituted benzene rings. We examine numerous example spectra and learn how the position of C-H wagging peaks, and the presence or absence of a ring-bending peak, allow one to distinguish between mono-, ortho-, meta-, and para-substituted rings most of the time.

Brian C. Smith

Structural isomers are molecules that have the same chemical formula but different chemical structures. Therefore, these molecules have different chemical properties such as boiling points and reactivities. Structural isomers have the same mass so they are difficult to distinguish by mass spectrometry. However, infrared (IR) spectroscopy, where the peak positions are determined by the atomic masses and bond strengths of the functional group undergoing vibration (1), can distinguish between structural isomers because each structural isomer has a unique set of masses and bond strengths.

In the last installment (2), I introduced the topic of aromatic bonding and aromatic rings, and we looked at the spectrum of the prototypical aromatic ring benzene in detail. In this installment, we expand our knowledge of the IR spectroscopy of aromatic rings by looking at the spectra of mono- and disubstituted benzene rings. There are three ways of arranging two substituents around a benzene ring, meaning that disubstituted rings have three structural isomers, hence the need for a discussion of structural isomers and substituted benzene rings in one article.

Structures of Mono- and Disubstituted Benzene Rings

Benzene has six hydrogens and each of them can be replaced with a substituent, meaning a benzene ring can have up to six substituents. However, most of the substituted benzene rings you will come across will have one or two substituents, referred to as mono- and disubstituted benzene rings, respectively. Figure 1 shows the chemical structures of these types of rings.

The monosubstituted molecule in Figure 1 is properly called methylbenzene, but most of us know it as toluene. As you can see, toluene simply consists of a methyl group attached to a benzene ring.

The three structural isomers of disubstituted benzene rings are named ortho-, meta-, and para-. Their structures are illustrated using the xylenes (or dimethylbenzenes) in Figure 1. Ortho-xylene has two methyl groups on adjacent carbons. Meta-xylene has two methyl groups separated by one carbon. In para-xylene the two substituents are across the ring from each other and there are two carbons between the methyl groups. I remember these substitution patterns by thinking of the letters OMP and recalling that the two substituents get further apart as one goes from ortho- to meta- to para-. To remember the letters OMP I use a silly chemical mnemonic like "Oh My Palladium."

The infrared spectrum of toluene is shown in Figure 2. Toluene contains unsaturated carbons in its benzene ring and a saturated carbon in its methyl group, making it a "mixed molecule." Recall (3) that unsaturated carbons generally have C-H stretching peaks above 3000 cm^{-1}, whereas saturated carbons have C-H stretches below 3000 cm^{-1}. Toluene conforms to this pattern with C-H stretches above and below 3000 cm^{-1} as denoted by the letter A in Figure 2.

Recall that ring modes are from the stretching of the carbon-carbon bonds in the benzene ring, that they vary in number and intensity, and fall between 1620 and 1400 cm^{-1} (2). Toluene's ring modes appear at 1604 and 1495 cm^{-1} as denoted by the letter B in the figure. The C-H wag, the most intense band in the spectrum, is seen at 728 cm^{-1} as denoted by the letter C. Previously I stated (2) that the C-H wags of benzene rings generally fall from 1000 to 700 cm^{-1}. However, we can be more specific with this peak's range. Benzene ring C-H wagging peak positions are sensitive to substitution pattern. For monosubstituted benzene rings such as toluene the C-H wagging peak falls between 770 and 710 cm^{-1}.

The second most intense peak in Figure 2, labeled D at 694 cm^{-1}, is new to us. The vibration giving rise to this peak is a ring bend. Imagine the carbon–carbon bonds in the molecule's benzene ring bending above and below the plane of the molecule. The beauty of this peak is that depending upon a benzene ring's substitution pattern it is both present and intense as seen in Figure 2, or completely absent. The presence or absence of this peak is determined by the symmetry of the substitution pattern, $d\mu/dx$ is either large or zero depending on whether the molecule is mono-, ortho-, meta-, or para-substituted. When it does appear, this ring bending peak falls at 690 ± 10 cm^{-1}. The key then to distinguishing a monosubstituted benzene ring is a C-H wag between 770 and 710 cm^{-1} and the presence of a ring bend near 690 cm^{-1}. As we will see, it is the position of the C-H wag and the presence or absence of the ring bending peak together that can be used to distinguish mono- and disubstituted benzene rings from each other.

The infrared spectrum of ortho-xylene is shown in Figure 3. Because this molecule has saturated and unsaturated carbons present, there are C-H stretching peaks above and below 3000 cm^{-1}, as denoted by the A label. The ring modes are at 1604 and 1495 cm^{-1}, which are labeled B. These ring-mode peak positions are identical to toluene, which is why ring modes should not be used to determine the substitution pattern around a benzene ring. The C-H wag in Figure 3 appears at 742 cm^{-1} as denoted by the letter C. For ortho-substituted rings in general this peak falls between 770 and 735 cm^{-1}. Note that there is no ring bending peak near 690 cm^{-1} in this spectrum, as is typical of ortho-substituted rings. Thus, there is only one diagnostic peak for ortho-substituted rings, the C-H wag.

In theory, one could confuse the spectra of mono- and ortho-substi-

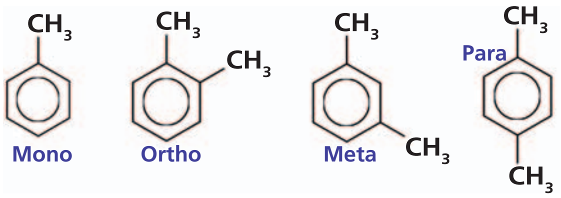


Figure 1: The chemical structures of mono-, ortho-, meta-, and para-substituted benzene rings, illustrated using toluene and the xylene family of molecules.

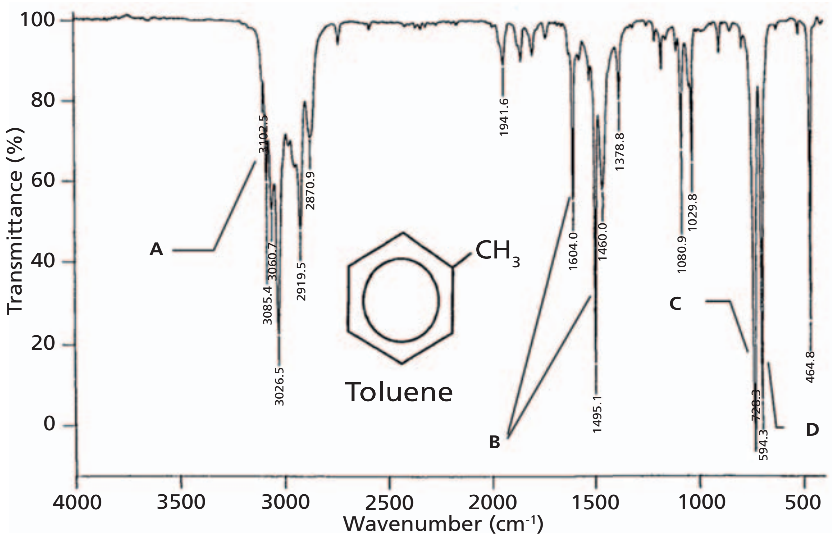


Figure 2: The IR spectrum of toluene, measured as a capillary thin film.

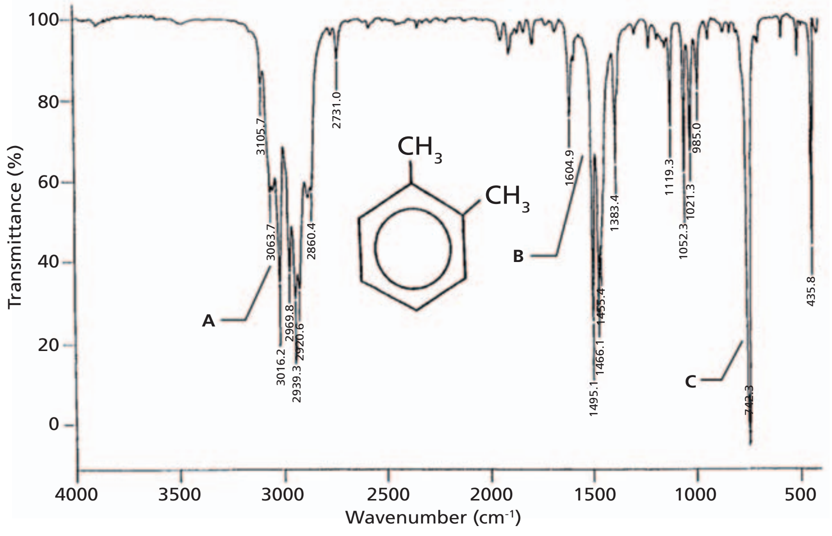


Figure 3: The IR spectrum of ortho-xylene, measured as a capillary thin film.

Quiz Section: Answer to the March Quiz and a New Interpretation Challenge

The Last Quiz

In the last installment (2), you were tasked with identifying the C-H stretches, summation bands, ring modes, C-H in-plane bends, and C-H wags for the spectrum shown in the figure to the right labeled "The last quiz." A list of the peaks in the problem spectrum is shown in the left column of the table below. I did not ask you to solve for the complete chemical structure of this molecule as we had not yet covered all the material needed for you to do so.

Correct peak assignments from the March 2016 problem	
3084, 3063, and 3027	Unsaturated C-H stretches
2968, 2931 and 2873	Saturated C-H stretches
1941, 1801	Summation bands
1604, 1495	Ring modes
1036, 1030	In-plane C-H bends
745	Out-of-plane C-H bend

The correct assignments of the relevant peaks in the problem spectrum are shown in the table above.

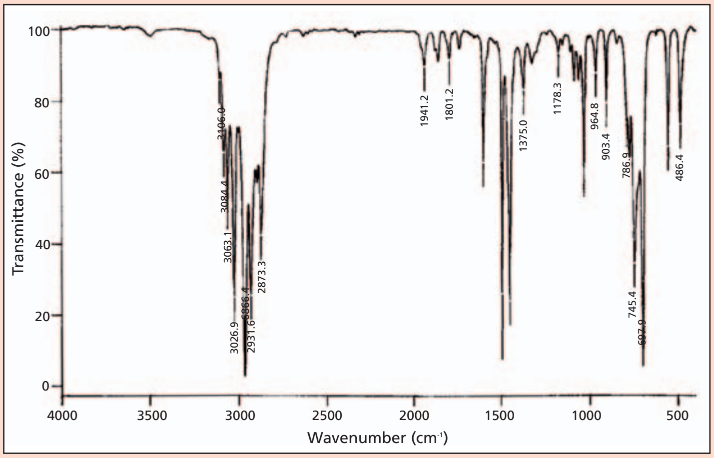
In the spectrum to the right there are peaks above and below 3000 cm^{-1}, thus this is a mixed molecule containing saturated and unsaturated carbons. Note that there are three saturated C-H stretches between 3000 and 2850 cm^{-1}. Recall from a previous column (3) that if there are three or more peaks in this wavenumber region that the molecule contains both methyl and methylene groups. Thus, the three peaks at 2968, 2931, and 2873 cm^{-1} are assigned as methyl asymmetric, methylene asymmetric, and CH_3 symmetric stretches, respectively. Also recall (3) that methyl groups have an "umbrella mode" C-H bending peak at 1375 ± 10 cm^{-1}. This peak appears exactly where it should in the figure and confirms the presence of the methyl functionality in this sample. Lastly, both CH_2 and CH_3 groups have a C-H bending peak around 1460 cm^{-1} (3). This peak is at 1453 cm^{-1}.

There is a series of four summation bands from about 2000 to 1700 cm^{-1}. Their significance will be discussed in a later column. The peaks at 1604 and 1495 cm^{-1} are ring modes. There are a couple of weak aromatic ring in-plane C-H bending peaks present in the problem spectrum, but these are not of much diagnostic utility. Recall (2) that aromatic ring out-of-plane C-H stretches (wags) fall between 1000 and 700 cm^{-1}. This peak is found at 745 cm^{-1}.

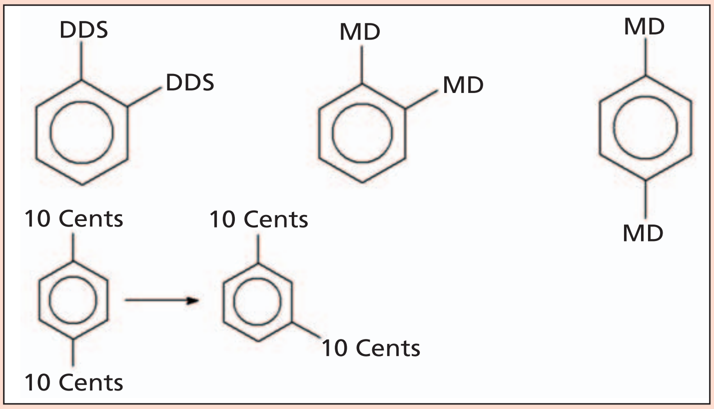
New Quiz

This column's quiz is a two-parter. Because some of you may be new to the naming of substituted benzene rings, some practice is in order. Using what you learned above, give the substitution pattern and attempt to name each of the "molecules" seen in the figure below (labeled "New quiz"). In the bottom of the figure there is a "chemical reaction"—try to name it if you can. (Hint: don't take this problem too seriously.)

The second and more serious part of this quiz is to finalize the identification of the molecule in the last problem. Its spectrum is shown below and its peaks are assigned in the table. You now know everything you need to know to discern the complete chemical structure of this molecule.



The last quiz: The problem spectrum from March 2016, the IR spectrum of a liquid.



New quiz: Name the "molecules" and "chemical reaction" in this figure.

tuted rings because their C-H wagging peak ranges overlap. However, the ring bend is clearly present in mono-spectra and absent from ortho-spectra, meaning that these two are actually easy to distinguish from each other.

The IR spectrum of meta-xylene is shown in Figure 4. Since meta-xylene is a mixed molecule, there are C-H stretches above and below 3000 cm^{-1} (labeled A). There are ring modes at 1612, 1591, and 1491 cm^{-1} denoted B, and the C-H wag is at 768 cm^{-1} labeled with a C. For meta-substituted benzene rings in general, the C-H wag falls from 810 to 750 cm^{-1}. The second most intense peak in the spectrum at 691 cm^{-1}, denoted with a D, is a ring bend. Ring bends for meta-substituted benzene rings appear in the same range as for monosubstituted rings, 690 ±10 cm^{-1}. Thus, the

Table I: Diagnostic bands for mono- and disubstituted benzene rings

Substitution Pattern	Out-of-Plane C-H Bending	Ring Bend (690±10 cm^{-1})
Mono	770–710 cm^{-1}	Yes
Ortho	770–735 cm^{-1}	No
Meta	810–750 cm^{-1}	Yes
Para	860–790 cm^{-1}	No

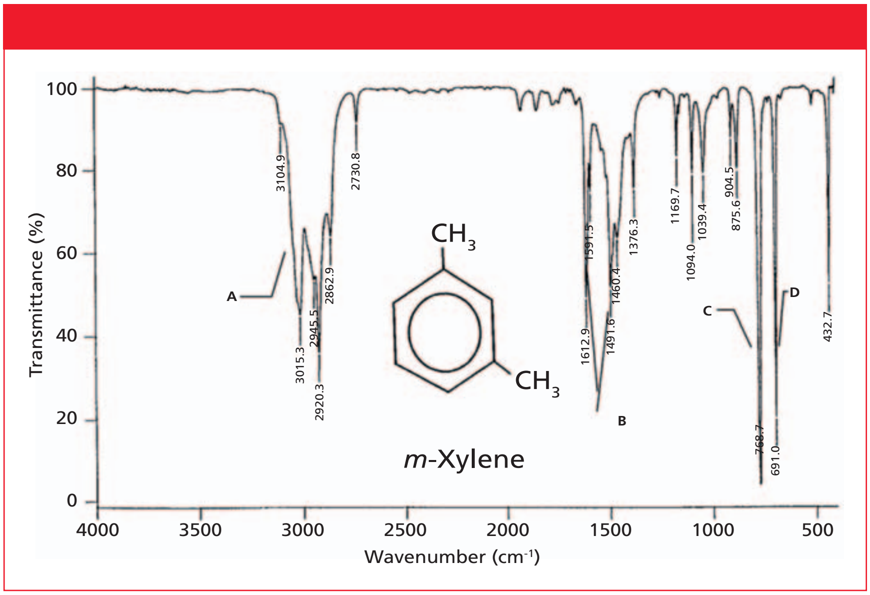


Figure 4: The IR spectrum of meta-xylene, measured as a capillary thin film.

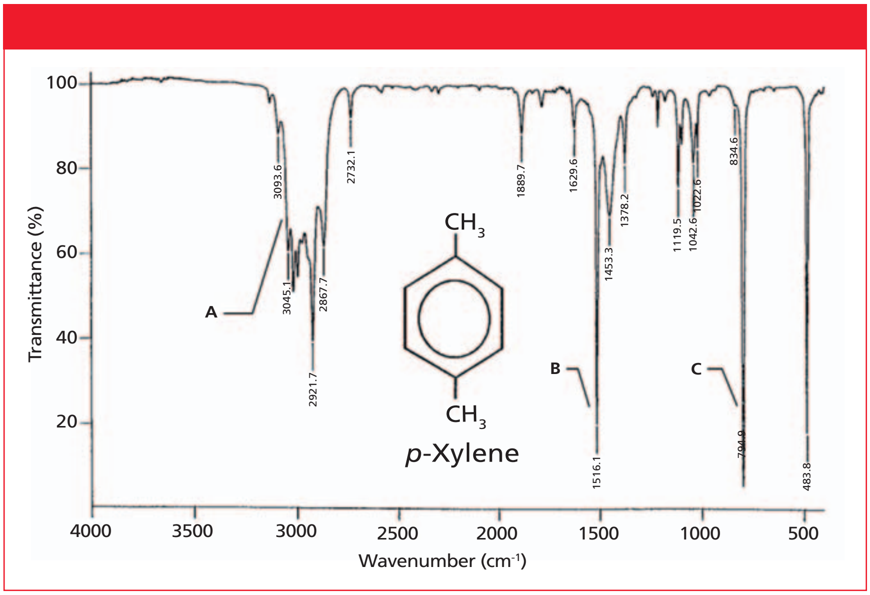


Figure 5: The IR spectrum of para-xylene, measured as a capillary thin film.

diagnostic peaks for meta-substituted rings are the presence of a C-H wagging peak from 810 to 750 cm^{-1} and the ring bending peak near 690 cm^{-1}.

The infrared spectrum of para-xylene is shown in Figure 5. As expected there are C-H stretches above and below 3000 cm^{-1} in this spectrum labeled A. There is a strong ring-mode peak at 1516 cm^{-1} denoted with a B, and the C-H wag is at 795 cm^{-1} as pointed out with a C. For para-substituted benzene rings, generally the C-H wag falls between 860 and 790 cm^{-1}. Note the absence of a ring bend, so the only diagnostic feature for para-substituted rings is a C-H wagging peak.

We have seen from four examples that the position of the C-H wag and the presence or absence of the ring bending peak together can be used to distinguish mono- and disubstituted benzene rings from each other. This information is summarized in Table I. If you look closely at this table you will notice that if the C-H wag falls between 770 and 750 cm^{-1} and there is a ring bend present then the molecule could be mono- or meta-substituted. There is a way to distinguish between these molecules in this situation using other information in the spectrum, which will be discussed in the next column.

References

(1) B.C. Smith, *Spectroscopy* **30**(1), 16–23 (2015).
(2) B.C. Smith, *Spectroscopy* **31**(3), 34–37 (2016).
(3) B.C. Smith, *Spectroscopy* **30**(4), 18–23 (2015).

Brian C. Smith, PhD, is a Senior Infrared Product Specialist for PerkinElmer, based in San Jose, California. Before joining PerkinElmer, he ran his own FT-IR training and consulting business for more than 20 years, and taught thousands of people around the world how to improve their FT-IR analyses and interpret infrared spectra. Dr. Smith has written three books on infrared spectroscopy: *Fundamentals of FTIR* and *Infrared Spectral Interpretation,* both published by CRC Press, and *Quantitative Spectroscopy: Theory and Practice* published by Academic Press. He has published a number of papers in peer-reviewed journals and is a co-inventor on a patent for an FT-IR method to monitor dust exposure in coal mines.

Review of New Spectroscopic Instrumentation for 2016

Our annual review of new spectroscopy products introduced at Pittcon or during the previous year.

Howard Mark and Mike Bradley

Here we present our annual review of new spectroscopy instruments, components, and accessories, including our assessment of what these new products reveal about instrumentation trends.

In the past, our annual review was restricted to products introduced at the Pittsburgh Conference (Pittcon). A few years ago, however, we began including products introduced independently of Pittcon, reflecting the fact that vendors are increasingly launching their products at a variety of conferences and trade shows and sometimes without any connection to an event. Thus, we are reviewing products released at Pittcon (the vast majority that appear here) as well as other products launched in the last 12 months.

For many reasons, Pittcon attendance has been decreasing in recent years. The attendance in 2016 was down more than 10%, with 12,841 official attendees (7374 conferees, 5082 exhibitors, and 385 other registrants) versus 14,272 in 2015. The exposition remains strong, with 846 exhibiting companies occupying 1538 booths (http://pittcon.org/exposition, click on “all exhibitors”). Out of all the exhibors, 129 companies were listed as being new to the show. (A full breakdown and comparison with previous Pittcon events is available at http://pittcon.org/exhibitor/pittcon-demographics/.) We note that this year Pittcon did not present the Editor’s Choice awards; we hope this program will return in the future.

The review that follows is organized alphabetically (with the exception of accessories and components, both of which appear at the end) and categorized by wavelength region or type of spectroscopy (that is, mid-infrared [mid-IR], X-ray, Raman, and so forth). This structure allows readers to compare instruments from different manufacturers, but it also sometimes classes handhelds with high-end research tools. The categories used to classify the products are

- Atomic spectroscopy
- Imaging
- Mass spectrometry (MS)
- Mid-IR spectroscopy
- Near-infrared (NIR) spectroscopy
- Nuclear magnetic resonance (NMR)
- Raman spectroscopy
- Software
- UV–visible spectroscopy
- X-ray
- Accessories
- Components

Some of these categories (such as imaging) did not appear in last year’s review, while others that appeared last year (fluorescence) are missing this year, reflecting the ebb and flow of product development emphasis. In our taxonomy, “accessories” and “components” are inherently very general categories. The dividing line is this: “Accessories” (such as a sampling device) are used *with* an instrument, whereas “components” (such as a laser source or detector) are *part of* an instrument. The “software” category is focused on software developed independently from instruments, rather than software built to drive a particular instrument.

The Broad Trends

Instrumentation is evolving to cover an ever wider array of scientific problems, with a lot of activity at two extremes: At one end, the position of high-end instrumentation remains solid—witness the increasing resolution of mass spectrometers. On the other end, routine and field analyses are increasingly being taken over by handheld or portable devices.

This latter trend was the topic of two sessions at Pittcon, one on portable spectrometers and another on spectrometers driven by cell phones—and even cell phones as spectrometers. Fourier transform infrared (FT-IR), Raman, laser-induced breakdown spectroscopy (LIBS), and even NMR and MS systems are finding their way into the smaller footprints. In this approach, the standard attached computer is being replaced by “smart” devices, where the sensing, control, and analysis (that is, what is the answer?) are contained within the sensor.

The resulting stand-alone devices are far less limited than one would expect. However, these devices are not competitive with their larger, benchtop cousins in terms of sensitivity, signal-to-noise ratio, analytical performance, or other specifications. For instance, the small-footprint NMR devices are not yet capable of two-dimensional (2D) NMR. A major driving force, noted in last year’s review, involves the “analyzer” class of devices, where a specific customer need is met by a dedicated device; whereas benchtop units typically strive for flexibility, the portables are drilling down to an analytical need. It is noteworthy that while many of these devices started with small start-up companies, many are now part of mainstream analytical companies (such as Ahura and PicoSpin at Thermo Fisher Scientific, SensIR at Smiths Detection, and A2 at Agilent Technologies).

Instruments are also evolving to detect components in even smaller sampling sizes. Microliter sampling is now easy (Thermo Fisher Scientific) and both Raman and IR have been coupled with atomic force microscopes. Commercial fluorescence microscopes offer single-molecule detection (SMD) capabilities, and recent work in academic circles promises a broader range of SMD tools within the next few years.

Some devices, such as diamond attenuated total reflection (ATR) accessories for FT-IR and handheld Raman instruments, were launched in 2016 by multiple vendors. Obviously, all identified the same market need. Whether the market will provide a sustainable customer base for so many different vendors with generally the same offerings is not yet clear.

The Products

Each section of the review includes a brief discussion of interesting new products in the category and any salient trends. The corresponding table lists all the products in the category, in alphabetical order, and summarizes unique features. As noted earlier, the accessories and components sections are not listed alphabetically this year; instead they appear at the end.

As in the past, it is inevitable that some categories include products that might arguably be classified elsewhere, especially in regards to accessories, components, and software. Even some hyphenated techniques, such as inductively coupled plasma–mass spectrometry (ICP-MS) could be listed in either location. In such cases, the authors respected the classification given by the manufacturer.

"Imaging" represents a unique challenge. All imaging instruments use some underlying technology to create the images. There were enough products identi-

Table I: Index of companies mentioned in this article

Company Name	Category Listed Under
1st Detect	Mass spectrometry
ABB	NIR
ACD/Labs	Software
Agilent Technologies	Atomic and mid-IR
Andor Technology Ltd.	Imaging
Anton Paar	Accessories
Apco Ltd.	X-ray
ASD Inc., a PANalytical company	Software
Autoscribe Informatics	Software
Avantes	Raman and UV–vis
BaySpec	Components, imaging, mass spectrometry, and Raman
Bio-Rad Laboratories	Software
BioTools	Accessories, mid-IR, Raman, and software
Block Engineering	Mid-IR
Bruker BioSpin	Imaging and NMR/ESR
Bruker Optik GmbH	Mid-IR
B&W Tek	Atomic, NIR, software, and UV–vis
Carl Zeiss Spectroscopy GmbH	UV–vis
Cerno Bioscience	Mass spectrometry
Claisse	Accessories
Clippard Instruments	Components
Cobalt Light Systems Ltd.	Raman
Cobolt	Components
Crystal IS	Components
Czitek	Accessories
Distek, Inc.	Accessories
Elemission	Atomic
Fiveash Data Management, Inc.	Software
Galaxy Scientific	NIR
Gasera	Mid-IR
GFS Chemicals, Inc.	Accessories
Glass Expansion	Accessories
Harrick Scientific	Accessories and software
Headwall Photonics	Accessories, components, and imaging
Hellma Axiom, Inc.	Accessories
Heuresis Corporation	X-ray
Horiba Scientific	Atomic and software
Ibsen Photonics	Raman
Inorganic Ventures	Accessories
Inrad Optics	Components
Ionbench	Accessories
Industrial Test Systems, Inc. (ITS)	UV–vis
International Light Technologies	UV–vis
John Wiley & Sons	Software
Kaiser Optical Systems, Inc.	Raman
Keit Spectrometers	Mid-IR
Latitude Compliance Services	Software
LTB Lasertechnik Berlin GmbH	Atomic
Magritek	NMR
Mettler-Toledo	UV–vis
Metrohm	Raman and software
Microcertec	Components
Middleton Spectral Vision	Imaging

Table I: Index of companies mentioned in this article (continued)

Company Name	Category Listed Under
MilliporeSigma	UV–vis
MS Noise	Accessories
Ocean Optics	Accessories and NIR
Ondax	Accessories
Optical Support, Inc.	Imaging
OptiGrate Corp.	Components
PANalytical	X-ray
PerkinElmer	Mid-IR and UV–vis
Polymer Char	Components
QMC Instruments	Components
Quantum Composers Inc.	Accessories and components
rap.ID	Atomic
Raptor Photonics	Raman
Real-Time Analyzers, Inc.	NIR
Renishaw	Raman
Rigaku Corporation	X-ray
RPMC Lasers Inc.	Components
Shimadzu Scientific Instruments	Atomic and NIR
Si-Ware Systems	NIR
Specac	Accessories
Spectral Evolution	NIR and UV–vis
Spectral Sciences, Inc.	Software
Spectro Analytical Instruments	X-ray
SpectroClick	UV–vis
Spellman High Voltage Electronics Corp.	Components
Spetec GmbH	Accessories
Starna Cells	Accessories
StellarNet	Accessories, NIR, and UV–vis
tec5USA	UV–vis
Technospex	Raman and UV–vis
Teledyne CETAC Technologies	Accessories
Teledyne Leeman Labs	Atomic
Texas Instruments	Components, NIR, and software
Thermo Fisher Scientific	Mid-IR, NIR, NMR, Raman, and UV–vis
Tiger Optics	NIR
Tornado Spectral Systems	Components
Viavi Solutions	NIR
WITec GmbH	Raman
Xia LLC	Accessories

fied as "imaging" to warrant a separate category this year, but some imaging instruments (such as Raman imaging instruments) will be found under the corresponding technology; readers will need to check both categories. Readers also can search by company name in Table I to see under which categories a given company's products are listed. A few products based on multiple technologies are listed in more than one category.

Atomic Spectroscopy

At a high level, the key evolution within atomic spectroscopy (Table II) appears to involve the incorporation of new technologies—such as light-emitting diodes (LEDs) into the same core instrument design. As another example of the incorporation of new technologies, Agilent's ICP-OES system uses a dichroic spectral combiner to run samples faster.

Looking at the other specific offerings this year, we see that four companies are offering LIBS instruments. Elemission's instrument can analyze rocks of any form and size, either clean or with dirt, water, and so forth, at 100 spectra/s. The instrument from LTB Lasertechnik Berlin GmbH has very high spectral resolution (50,000 over the range 250–900 nm). B&W Tek has launched a handheld LIBS instrument. A new product from rap.ID combines LIBS with optical microscopy.

Horiba is showing two novel technologies. Its innovative glow-discharge instrument measures layer thickness and crater depth. The company also has a nondispersive analyzer for carbon and sulfur. Shimadzu has an ICP-MS instrument with reduced gas consumption. Teledyne Leeman Labs provides an ICP-OES instrument for environmental applications. Agilent's ICP-MS system includes optimization tools to simplify method development and operation.

Imaging

In previous years, a paucity of imaging products prevented our including this section in our review. Activity in 2016 enables us to reinstate this section (Table III).

The term *imaging* can be applied to many fields, including visible image collection, spectroscopy, and NMR. The result is a hypercube of data, often including spatial relationships. Visible imaging, especially for use in unmanned aerial vehicles (UAVs), now commonly known as *drones*, was specifically mentioned (by Headwall Photonics and BaySpec). This is a first step, we think, because the combination of handheld technology, imaging technology, and UAV operations should lead to increasingly sophisticated, low-cost, environmental monitoring tools. Aircraft do this already, but now tools are coming on-line for cost-effective UAV mounting. Wastewater effluent tracking and deforestation are two other exciting applications for this combined technology.

Andor showed an ultrafast platform for nanosecond time-resolved imaging and spectroscopy, using a unique combination of frame rates from 40 up to 4000 fps with better than 2-ns gating. Bayspec provides push-broom and snapshot models of high-performance mobile systems. Headwall Photonics has a unit designed for image collection from airborne platforms.

Middleton showed a combined hyperspectral and fluorescence imager. Optical Support presented a near-IR fluorescence system. Bruker BioSpin manufactures a magnetic resonance imaging (MRI) device with a 3-T magnet.

Mass Spectrometry

We received very few submissions for the MS category (Table IV), although MS is a popular and highly competitive market space. The likely explanation is that the major instrument companies that manufacture these complicated and expensive instruments primarily launch them at the Annual Conference on Mass Spectrometry and Allied Topics (ASMS) or other mass spectrometry conferences and did not submit forms for us to consider them for this review.

Thus, we have two products to include in this category this year. In connection with portability of instruments, Bayspec has a mass spectrometer that can be carried by one person. Cerno Bioscience provides a mass spectrometer with sub-part-per-million mass accuracy.

Mid-IR

Most of the new FT-IR products (Table V) match the theme we identified involving tools for specific types of analysis. Some new products were highly application-specific: Biotools launched a protein structure analyzer, optimized for that application. Block Engineering combines a mid-IR laser spectrometer with photoacoustics for a sensitive multigas analyzer. Bruker Optik has a gas analyzer for monitoring smokestacks, auto exhaust, and more. Gasera also has a photoacoustic gas analyzer for trace gas monitoring. Others involved general purpose FT-IR devices designed to be incorporated into process control or other specific applications: Keit manufactures a rugged, no-moving-parts spectrometer for direct insertion into production equipment. Thermo Fisher Scientific provides a gas analyzer to fit into a standard 19-in. rack. PerkinElmer manufactures an instrument designed for scientists in academia, pharmaceuticals, and more.

Agilent provides a mobile device with minimum weight (5 lb) and other characteristics to enhance the user experience.

With the horsepower race (signal-to-noise ratio) in mid-IR having reached limits beyond what most normal applications require, the main developments in this area appear to be related to usability and software tools. Usability improvements included a sample compartment microscope (Czitek) and new accessories (Harrick, Specac). Software is discussed in a separate section below, but we note here that the instrument control interfaces for many vendors are changing, driven by both customer expectations (the cell phone experience) and software platform obsolescence.

NIR

NIR Trends

The general trend in NIR instrumentation (Table VI), which started slowly a good while back and has been growing steadily since, is for manufacturers to provide instruments precalibrated for specific commodities or ingredients

Table II: Atomic spectroscopy products

Company Name	Product Name	Product Type	Measurement Mode	Applications and Unique Features
Agilent Technologies	Agilent 5100	ICP-OES	N/A	Can run samples up to 55% faster, using 50% less gas. Requires only one sequential measurement per sample, using the company's Dichroic Spectral Combiner and Synchronous Vertical Dual-view technologies.
	Agilent 7800	ICP-MS	N/A	Provides a wide dynamic range and excellent matrix-tolerance and interference removal. Optimization tools simplify method development and operation. Industry-specific application packages are available.
B&W Tek	NanoLIBS	Handheld LIBS spectrometer	N/A	A state-of-the-art handheld LIBS instrument for identification and investigation of raw materials including ionic salts such as NaCl and KCl. Can be used by nontechnical users to rapidly identify samples in the laboratory, warehouse, loading dock, or field.
Elemission	Mission: Rocks	LIBS, AES spectrometer	N/A	Can analyze rocks of any form and size; dry, clean, and in the presence of dirt or water. Analysis rate is 100 measurements per second.
	Mission: Sort	LIBS, AES spectrometer	N/A	Can sort metal scrap at a rate of up to 5 metric tons per hour. Real-time process monitoring to identify critical-to-quality and critical-to-yield parameters.
Horiba Scientific	DIP (Differential Interferometry)	Differential interferometry profiling for GD-OES	N/A	Patented DIP innovation for depth profiling by glow discharge optical emission spectrometry (GD-OES). DIP provides real-time layer thickness, crater depth, and sputter rate.
	EMIA Pro	Carbon–sulfur analyzer (NDIR)	N/A	Carbon–sulfur nondispersive infrared (NDIR) analyzer offers optimized for the range of 1.6 ppm–6.0% for carbon, and 2 ppm–1.0% for sulfur. The analyzer is equipped with a unique CO detector and a new cleaning mechanism that has improved cleaning efficiency compared to that of other carbon–sulfur analyzers.
LTB Lasertechnik Berlin GmbH	Aryelle 400	LIBS, AES spectrometer	N/A	Aryelle 400 in combination with a 2048 × 2048 pixel scientific-grade CCD detector provides resolving power of 50,000 over the 250–900 nm wavelength range and 15,000 for the 190–900 nm range.
rap.ID	Single Particle Explorer	LIBS in an optical microscope	N/A	LIBS integrated into an optical microscope. Image-directed spectroscopy delivers elemental composition in minutes. Can analyze microparticles, layered materials, coatings, and small inclusions. LIBS removes the top layers (3–10 μm) of sample within microseconds.
Shimadzu Scientific Instruments	ICPMS-2030	ICP-MS	N/A	Low gas consumption. Compatible with lower purity (99.95% pure) argon. Collision cell achieves high molecular ion elimination and high transmission efficiency. Can measure all elements without discharging the cell gas. Offers assistant software functions.
Teledyne Leeman Labs	Prodigy Plus	ICP-OES	N/A	Applications where elemental determinations are required such as in environmental, QA and QC, research, petroleum, pharmaceutical, nuclear, and chemicals.

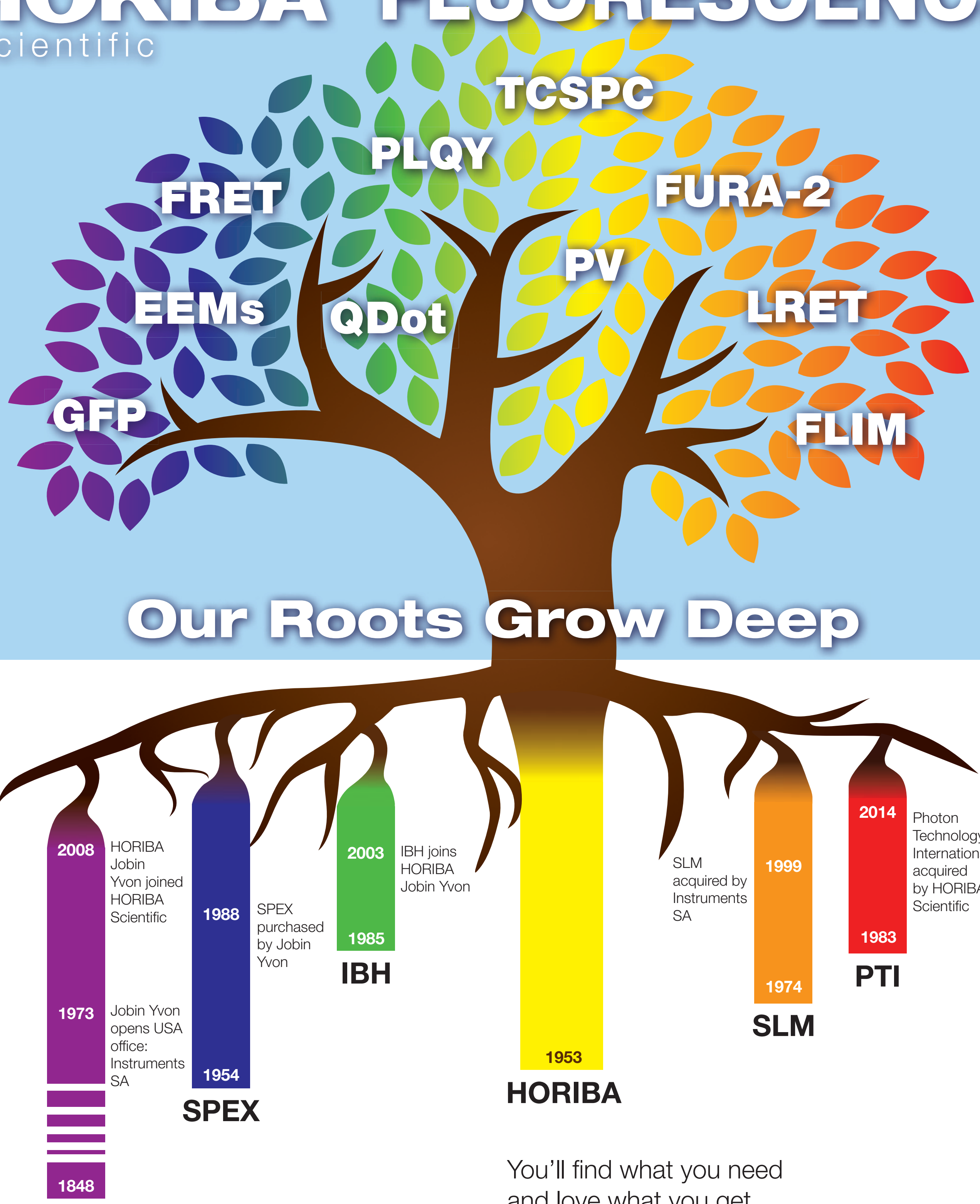
N/A = not applicable

that their customers want to measure. This would remove one of the biggest impediments to selling NIR instrumentation: the need for development of a calibration around new products and analyses. Specific analyzers allow users to perform additional analyses, often with lower total costs and much faster implementation. Increasingly, the value is driven less by hardware—which is often already good enough—than by the sets of calibration models that the manufacturer can supply to the user. Sometimes these new calibration models are offered in conjunction with extra algorithmic capabilities, but often they are simply adjunct to the algorithms already available.

Driven by this analyzer market, NIR products have been evolving quickly toward smaller sizes. This is most obvious from the number of handhelds appearing each year, with slightly different value propositions and performance, but with the same end goal of supplying a simple tool for a targeted analysis. Benchtop instruments are also coming down in size and cost. We are currently seeing components like broadband LED sources and specialized detectors driving this trend, and the increase in specialized detectors and sources we note in the components section will accelerate this move into even more specialized niches.

HORIBA FLUORESCENCE

Scientific


TCSPC

PLQY

FRET

FURA-2

PV

EEMs

QDot

LRET

GFP

FLIM

Our Roots Grow Deep

JY
1848
1973 Jobin Yvon opens USA office: Instruments SA
2008 HORIBA Jobin Yvon joined HORIBA Scientific

SPEX
1954
1988 SPEX purchased by Jobin Yvon

IBH
1985
2003 IBH joins HORIBA Jobin Yvon

HORIBA
1953

SLM
1974
1999 SLM acquired by Instruments SA

PTI
1983
2014 Photon Technology International acquired by HORIBA Scientific

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Table III: Imaging products

Company Name	Product Name	Product Type	Measurement Mode	Applications and Unique Features
Andor Technology Ltd.	iStar sCMOS	Ultrafast imager	Optical emission, fluorescence/photoluminescence, absorption, scattering (such as Raman)	Ultrafast platform for nanosecond time-resolved imaging and spectroscopy. Unique combination of frame rates up to 40 fps (4000 with ROI), better than 2-ns gating, high sensitivity Gen 2 and 3 image intensifiers and integrated high-resolution triple-output digital delay generator. Dual-frame mode available with optical inter-frame down to 100 ps for ultrafast flow PIV-type applications.
BaySpec	OCI	Ultracompact hyperspectral imagers	Reflection	High-performance mobile HSI system. Push-broom and snapshot models available. Random-speed sample scanning by push-broom; HSI cube generation by snapshot imagers.
Bruker BioSpin	BioSpec 3T	MRI imager	N/A	Translational field of 3-T, multipurpose, preclinical MRI and MRS systems. Bridges the gap from reference imaging at 1 T to research-level MRI imaging at high-field. Cryogen-free design eliminates liquid helium or nitrogen; magnet hold time of 4 h.
Headwall Photonics	High-Resolution Hyperspectral sensor	Hyperspectral image sensors	Reflection	Collect data from airborne platforms such as satellites and aircraft, for precision agriculture, crop science, environmental monitoring, infrastructure inspection (pipelines, dams, railroads), pollution mitigation, gaseous detection, and geology.
Middleton Spectral Vision	macroPhor	Push-broom fluorescence and NIR imaging	Reflection	Combines hyperspectral and fluorescence imaging. Other fluorescence spectrometers only acquire spectra over a limited area of the sample. Uses push-broom hyperspectral imaging to scan the image for both spatial and spectral information, providing the user with all the spectra for each pixel over the entire image.
Optical Support, Inc.	Near IR Fluorescent Imaging systems	Engineering design and manufacturing Services	N/A	OSI has machining, cleanroom, alignment, and test capabilities vertically integrated to provide prototyping and manufacturing. Expertise in optical and mechanical design and who need to validate design and volume production.

N/A = not applicable

Table IV: Mass spectrometry products

Company Name	Product Name	Product Type	Measurement Mode	Applications and Unique Features
BaySpec	Portability	Mass spectrometer	N/A	Carried by one person for in-situ and direct analysis techniques. Can sample solid, liquid, and gas samples from atmosphere.
Cerno Bioscience	Best Scan sCLIPS	Mass spectrometer	N/A	1–2 ppm or even sub-part-per-million mass accuracy, in high-resolution MS systems; additional isotope information must sometimes be used. Provides the only solution available to evaluate each scan for best possible elemental composition determination.

N/A = not applicable

New NIR Products

ABB offers in-line monitoring and control of continuous processes. B&W Tek's instrument has a capability of combining NIR with UV–vis measurements. Galaxy Scientific improves the analytical results of its portable instrument by having permanently aligned optics. Viavi has an ultracompact instrument made for maximum portability. Ocean Optics offers high performance at a low price using uncooled InGaAs array detectors that can also measure and report transmission, absorbance, reflectance, color, radiometer, solar measurement fluorescence, Raman spectroscopy, and radiometery. Spectral Evolution also has a field-portable radiometer with no moving optical parts.

Several manufacturers launched tools for dedicated applications this year. Real-Time Analyzers offers a tool that can determine fuel quality as well as chemical and physical properties of multiple diesel, gasoline, jet fuel, and so forth, using transmission. Thermo Fisher Scientific addresses routine analysis with transmission and reflection measurement capabilities. Shimadzu offers functional NIR (fNIR) for blood oxygen and other medically-important analyses.

Several offerings in this category were aimed at original equipment manufacturers (OEMs). Stellarnet has an instrument for OEMs and sensing applications. Texas Instruments also addresses OEMs with the TI DLP technology that uses single-element InGaAs detectors. Si-Ware offers the most compact and lowest-cost FT-IR system available. Tiger Optics mea-

Table V: Mid-IR products

Company Name	Product Name	Product Type	Measurement Mode	Applications and Unique Features
Agilent Technologies	Agilent 4300	Handheld FT-IR spectrometer	ATR, diffuse reflection, external reflection, grazing angle, germanium ATR	Accurate, nondestructive molecular analysis. Weighs less than 5 lb, for mobile measurement. Interchangeable interfaces. Optimized electronics and ultrashort internal optical path. Includes intuitive mobile software, no alignment optics, one-button method initiation, and automatic interface.
	Agilent Cary 610	FT-IR microscope	ATR	Designed to provide clear, highly detailed images in minutes.
BioTools	PROTA-3S	FT-IR protein structure analyzer	Transmission	Combines speed, sensitivity, and simplicity for fast, accurate results. Rapid measurements: 1–2 min collection, low concentration capability (less than 0.25 mg/mL), no limit on high concentration.
Block Engineering	LaserSense-PA	Combined mid-IR and photoacoustic spectrometer	Transmission	Uses both mid-IR laser and photoacoustic technologies for multigas analysis. Sensitivities from parts-per-billion to percent levels. For in-line process monitoring and control and point detection.
Bruker Optik GmbH	Matrix-MG	Mid-IR spectrometer	Transmission	Quantification of gases in complicated mixtures: monitoring production lines in industrial applications, monitoring exhaust gas of smokestacks, analysis of motor vehicle exhaust, biogas analysis, determination of gas impurities, and scientific research.
Gasera	Gasera One	Photoacoustic mid-IR gas analyzer	Photoacoustic mid-IR	Trace-level monitoring of toxic and harmful gases. Uses cantilever-enhanced photoacoustic detection technology, combined with several infrared light sources for reliable parts-per-billion-level trace gas monitoring. Requires no consumables and has a long calibration interval and easy-to-use user interface.
Keit Spectrometers	microFTS	FT-IR spectrometer	ATR and transmission accessories	A compact, rugged and vibration-proof FT-IR spectrometer. No moving parts, making it shock proof and suited for the production environment. Inserts directly into production equipment, eliminating the need for fiber-optic cables, remote sampling, and frequent recalibration, thus enabling faster decisions with real-time reaction monitoring.
PerkinElmer	Spotlight 150i/200i	Mid-IR spectrometer	N/A	Designed for scientists in materials, pharmaceuticals, academia, forensics, biomedical, and biomaterials applications
Thermo Fisher Scientific	Nicolet iG 50 FT-IR Spectrometer	FT-IR spectrometer	Transmission	Fits into a standard 19-in. rack. Applications: Routine gas, liquid, and film analysis for industrial process monitoring, continuous monitoring of gas emissions, and chemical or polymer process monitoring.

N/A = not applicable

sures various gaseous components to parts-per-billion levels.

NMR and ESR

As seen last year, there are only a few vendors working with NMR (Table VII), and the key innovations are primarily aimed at the benchtop instrument market. The high-end market largely belongs to one major vendor (Bruker), but several companies (such as Bruker, Magritek, and Thermo Fisher Scientific) delivered small-frame instruments based on permanent magnets, now that advances in materials have reached the point where permanent magnets of adequate strength and uniformity are possible. The original evolution of this, exemplified by the PicoSpin products (now Thermo Fisher Scientific), involved moderately performing instruments designed to give only the simplest of answers. Competition is now driving improved specifications and higher field magnets with more sensitivity. Most vendors this year introduced a reaction monitoring application, where the specificity of NMR is harnessed to provide insights into reacting mixtures and industrial processes.

The long-range evolution of NMR will be limited only by the field strength of the magnets and the stability of the fields generated. Pulse sequences and two-dimensional transforms are already implemented on high-field devices, so improved magnets could bring these techniques onto the benchtop in the not too distant future.

Bruker's Biospin offers benchtop systems with novel solutions (including a dedicated food analyzer) and dedicated software. Magritek also has a benchtop instrument without cryogens or needing to spin the sample. An instrument from Thermo Fisher Scientific requires only a 40-μL sample, and the instrument can be hand-carried.

Raman

We would argue, based on what we have seen preparing this review, that no other product line has shown a greater number and variety of tools coming into the market than Raman spectroscopy (Table VIII). There are two broad classes of tools: the large, benchtop instruments (such as those products launched by BaySpec, Renishaw, Thermo Fisher Scientific, and WITec) and the handhelds (such as those launched by BaySpec, BioTools, Metrohm, and Thermo Fisher Scientific).

Table VI: NIR products

Company Name	Product Name	Product Type	Measurement Mode	Applications and Unique Features
ABB	TALYS ASP400-Ex	Fiber-optic analyzer	Transmission	In-line monitoring and control of continuous processes. Features include simple installation and operation, small footprint, embedded controller, virtually no scheduled maintenance for 5 years.
B&W Tek	iSpec25	Portable UV–vis-NIR spectrometer	Diffuse reflectance	A broadband portable spectrometer reflectance probe for measurements from 350 to 2500 nm. Contains Si, InGaAs, and extended InGaAs arrays for optimal sensitivity and dynamic range. iSpec 4 software provides control and data collection for multiple spectrometers.
Galaxy Scientific	QuasIR	Portable FT-NIR analyzer	Transmission and reflectance	A dual-beam version of the company's Concavus spectrometer. Spectral resolution is 0.22 NA, and athermal characteristics of less than 0.15-nm wavelength shift over the 10–50 °C temperature range. The dual-beam spectrometer compensates lamp intensity fluctuation in real-time. The system uses a single concave grating for both beams and exhibits very low stray light. Can be customized for OEM use.
Ocean Optics	Flame-NIR Spectrometer	Flame-NIR spectrometer	Absorbance, transmission, reflectance, irradiance, emission	Costs about one-fourth that of a traditional NIR system. Flame-NIR pairs a high-performance uncooled InGaAs array detector with a small optical bench. Also uses a diode-array detector for high sensitivity from ~950 to 1650 nm, high thermal stability, and low unit-to-unit variation.
	NIRQuest Spectrometer	NIR spectrometer	Transmission, absorbance, reflectance, color, radiometer, solar measurement fluorescence, Raman spectroscopy, radiometry, chemistry	A robust, reliable spectrometer with a fast response time and good optical resolution over 900–2500 nm. NIRQuest has upgraded its optical bench with a replaceable slit design as a standard feature and an internal shutter as an option, which helps to mitigate some of the trade-offs associated with fixed-slit optical bench designs and applications where shuttering is integral to effectively managing light throughput in the spectrometer.
Real-Time Analyzers, Inc.	Portable Fuel Property Analyzer	NIR spectrometer	Transmission	Able to determine fuel quality and chemical and physical properties of diesel, gasoline, and jet fuel in less than 10 s.
Shimadzu Scientific Instruments	LABNIRS	Functional NIR spectroscopy (fNIRS) system	Functional NIR spectroscopy (fNIRS)	For brain imaging, multichannel, high-sensitivity optical blood oxygen level dependent (BOLD) imaging. Systems configured with up to 142 channels.
Si-Ware Systems	NeoSpectra SWS62221	Portable FT-IR spectrometer	Transmission and reflection	The most compact and lowest cost FT-IR spectral sensor available. It has three wide spectral ranges, depending on the configuration, from 1150 to 2500 nm. Constructed from low-cost, permanently aligned, and highly reproducible components for portability and easy integration.
Spectral Evolution	PSR+	Field spectroradiometer	Transmission, reflectance, absorbance	High-resolution, high-sensitivity, lightweight, field-portable spectroradiometer with no moving optical parts. Sealed unit. Fast, accurate in situ measurement of NIR spectra.
	RS-3500	Remote sensing bundle	Transmission, reflectance, absorbance	High-resolution, high-sensitivity, lightweight, portable, fiber optic spectroradiometer plus accessories for remote sensing.
StellarNet	RED-Wave	Micro NIR spectrometer	MEMS-based Fabry-Pérot tunable filter	Designed for OEM and sensing applications in NIR. This miniature spectrometer covers spectral regions where InGaAs detector array technology lacks sensitivity.
Texas Instruments	TI Design TIDA-00554 – DLP	Ultramobile spectrometer for portable chemical analysis with Bluetooth connectivity	N/A	Reference design TIDA-00554 uses TI DLP technology with a single-element InGaAs detector for portable high-performance measurements. More affordable than an array or gratings. Supports Bluetooth for handheld spectrometers. Developers can create their own data collection and analysis.
Thermo Fisher Scientific	Nicolet iS 5N	FT-IR	Transmission, reflection	Routine analysis in the NIR spectral range. Suggested applications: hydroxyl values and biodiesel blend ratios.

Table VI: NIR products (continued)

Company Name	Product Name	Product Type	Measurement Mode	Applications and Unique Features
Tiger Optics	ALOHA+ H_2O	Moisture analyzer	Transmission	2 ppb detection capability in ammonia (NH_3) and sub-part-per-billion in inert matrices.
	HALO OK	Oxygen analyzer	Transmission	Trace-level oxygen analysis: Parts-per-trillion detection capability, speed of response, wide dynamic range, absolute measurement, low maintenance, and low cost of ownership.
	Spark Dewpoint	Moisture–dewpoint analyzer	Transmission	Automatic verification and zeroing. No consumables or calibration gases required. Drift-free performance. Huge dynamic range: –100 to –13 °C.
Viavi Solutions	MicroNIR OnSite	NIR spectrometer	Reflection	Ultracompact NIR sensors and analyzers. Low weight (<3 lb), battery-powered, and equipped with WiFi connectivity.
	MicroNIR	PAT NIR spectrometer	Reflection	Weighs less than 3 lb, battery-powered, WiFi connectivity, suitable for in-line process monitoring. Covers the wavelength range of 950–1650 nm.

N/A = not applicable

Table VII: NMR and ESR products

Company Name	Product Name	Product Type	Measurement Mode	Applications and Unique Features
Bruker BioSpin	InsightMR	Flow tube and dedicated software	NMR	For real-time online monitoring by NMR. Compatible with any Bruker 5-mm probe; high pressure capability (over 10 bar), temperature-regulated transfer lines.
	Food Screener	NMR spectrometer	NMR	NMR spectrometer based on 400-MHz, simultaneous identification quantification of compounds, reduced cost per sample, screening method for targeted and nontargeted analyses, detection of unexpected and unknown fraud, analysis of origin authenticity, purity, false labeling, production process control, and sample similarity. Results are laboratory-, user-, and system-independent.
	EMX Nano	ESR spectrometer	Continuous wave	Benchtop system, motorized integrated field and amplitude reference standard, work-flows for data acquisition and analysis. Fully calibrated for quantitative analysis, software module for concentration determination, software module for spectrum fitting and identification. Integrated spectrum library.
Magritek	Spinsolve	60-MHz benchtop NMR spectrometer	NMR	60-MHz NMR spectrometer designed to deliver high resolution and sensitivity in seconds at the laboratory bench. No spinning, benchtop size and weight, no cryogens. Uses the company's patented Halbach magnet technology. Available for proton–fluorine or proton–fluorine–carbon with others to be added.
Thermo Fisher Scientific	picoSpin	Series II NMR spectrometer	N/A	40-µL flow-injection sample introduction via a handheld syringe or a pump. Glass NMR tubes not required. Can be hand-carried from the classroom to the laboratory. Rapid stabilization before data collection.

N/A = not applicable

The benchtop instruments stress spatial resolution (sub-1-µm), polarization, and high-speed imaging enabled by electron multiplying charge coupled devices (EMCCDs). These instruments are aimed at the materials sciences and research markets.

Meanwhile, the handheld market is being driven by the availability of small, lower-power consumption lasers, miniature monochromators, and polychromators and detectors (see the component section). Here the commercial role is materials identification, where vendors speak of penetration through glass and plastic containers, insensitivity to water (one bane of infrared), and answers consisting of identification rather than just spectra.

In both cases, a major competitive edge is claimed based on software. The ability to collect the data is similar—the manufacturers are all using similar components—so the differentiation comes in the user experience. Researchers who like to tinker can find open tool sets while a user seeking a simple answer (to a question such as, “Is the sample safe or dangerous?”) can get it. There is much debate over which laser works best, or whether a front-illuminated EMCCD is better than a rear-illuminated one, but most users will see the software and automation as key decision points.

Raman will continue to change rapidly, we feel, as it becomes embedded in both industrial processes and hyphenated research tools, such as rheometry–

Raman. This trend toward ongoing change will be driven by further developments in the components and software tools driving them.

Configurable for Dedicated Applications

Many new products this year are configurable for dedicated applications. Avantes customizes the instrument to the application by bundling software, probe, and application-specific recommendations. Raptor Photonics has a configurable instrument with a choice of sensors, coatings, windows, cooling options, and interface for OEM use. BaySpec directs various instrument models to different types of applications by emphasizing different characteristics: ruggedness, precision measurements, or microspectroscopy. Ibsen Photonics also offers a ruggedized instrument.

BioTools offers a 532-nm laser, an unconventional laser for handhelds, with tools to minimize the impact of fluorescence. Cobalt Light has spatially offset capability for its Raman instrument. Technospex combines Raman, photoluminescence, and laser-induced fluorescence in one instrument. Kaiser Optical provides high-resolution, research-grade Raman spectra on a portable platform. WITec provides a confocal micro-Raman system for 2D and three-dimensional (3D) analysis of the smallest sample volumes. Metrohm uses a laser with a Class 1 safety rating and orbital raster scanning. Renishaw uses feedback to follow the height of the sample. Thermo Fisher Scientific offers submicrometer resolution images for morphological and structural information.

Software

Software (Table IX), in the context of this review, consists of several different types of products. The first type consists of actual computer programs: the sequences of instructions that computers use to carry out their functions. The second consists of various types of data. One important subcategory of the latter consists of actual databases: sets of related data that can be used in a manner similar to dictionaries or encyclopedias—as compendia of important facts and relationships among those facts. A third type of product that we would include under the "software" heading is somewhat unique to the fact that spectroscopy is heavily dependent on chemometric algorithms; this third type of software consists of the models or collections of models (a "database" of models) that can be used by the chemometrics algorithms to analyze future samples; many of these, however, are unique to a particular manufacturer's spectrometers. This category tends to be promoted by instrument manufacturers to further their interest in selling instruments without requiring users to calibrate them. The final type of software is not readily definable, but consists of a miscellaneous group of offerings that provide something other than hardware (for example, nondigitized spectral libraries).

Software continues to respond to—and indeed to some extent, guide—the evolution of the laboratory requirements. Several vendors released software targeting specific applications (such as Bio-Rad, BioTools, and Texas Instruments), while others (such as ACD/Labs and Autoscribe Informatics) released products targeting information from spectra to sales team training. In the instrument field, software is often released in conjunction with instrument releases (seen in the examples of Texas Instruments and Harrick Scientific). Increasingly, the line between hardware-driven specifications (like signal-to-noise ratio) and software specifications (such as multicomponent searching) is being blurred in the competitive landscape, as vendors recognize and respond to specific customer demands. In many applications, spectra are no longer shown; just search or quantitative results are shown. Large databases (such as those offered by Bio-Rad and Fiveash Data Management) are also available; without these, the searching algorithm is like an empty box.

Based on discussions we had with vendors at Pittcon, it appears that the future of spectroscopy software will hold increased cloud computing and data storage, although data security and integrity continue to be major concerns (especially in the pharmaceutical industry). Simultaneously, the power of stand-alone instruments with built-in computing and analysis software is increasing, especially in handhelds but also in small benchtop instruments.

Integration Products

ACD Labs provides software to combine spectra and data from different techniques for simultaneous analysis. ASD's offering can collect data from two instruments simultaneously to allow

Table VIII: Raman products

Company Name	Product Name	Product Type	Measurement Mode	Applications and Unique Features
Avantes	AvaRaman Bundles	Raman spectrometer	Raman scattering	Bundles software and probe with application-specific recommendation for spectrometer. For laboratory analysis and process applications, including mineralogy and gemology; raw materials identification; pharmaceuticals and medical diagnostics; and semiconductors.
BaySpec	Agility	Dual-band portable Raman spectrometer with active trigger	Raman scattering	High sensitivity and repeatability, ruggedized, battery-operated package. Available in 532-, 785-, and 1064-nm versions.
	Nomadic	HR– mutli-laser confocal Raman microscope	Raman scattering	f/2 volume phase grating (VPG) technology, ultrafast electronics, deep-cooled CCD, and InGaAs detectors. Consists of a dedicated spectrometer for each laser excitation. 1064-nm Raman often overcomes fluorescence background.
BioTools	RamTest	Raman spectrometer	Raman scattering	Handheld Raman with 532-nm laser excitation with tools to minimize the impact of fluorescence. Lower instrument cost, up to 5–16 times faster analysis, widest in-class spectral range (120–4000 cm^{-1}), spectral resolution of 4–6 cm^{-1}.
Cobalt Light Systems Ltd	Resolve	Spatially offset Raman spectrometer	Spatially offset Raman spectroscopy (SORS)	Enables true through-barrier hazardous and contraband materials identification; a new handheld capability for hazmat, EOD, and search or law enforcement. Identifies materials through nonmetallic barriers such as colored plastics, glass, wrapping, paper, card, sacks, and fabrics.
Ibsen Photonics	EAGLE Raman-S	Raman spectrometer	N/A	Provides high sensitivity, wide range, and high resolution in a compact, ruggedized form. This is accomplished with fused-silica, surface-etched transmission gratings for wider wavelength range and higher efficiency grating technology.
Kaiser Optical Systems, Inc.	Raman-Rxn2	Multichannel analyzer	Raman scattering	Provides high-resolution, research-grade Raman spectra on a portable platform. One analyzer can collect Raman data from four channels, addressable by fiber-optic probes, and capable of direct in situ liquid or solid measurements.
Metrohm	MIRA (Metrohm Instant Raman Analyzer)	Raman analyzer	Vial holder or point-and-shoot	Handheld Raman instrument has a class I laser safety rating and orbital raster scanning (ORS) technology. Includes three quick-change inserts for point-and-shoot operation.
Raptor Photonics	Toucan	Raman spectrometer (kit)	N/A	Spectroscopy OEM CCD platform offers a choice of sensors, coatings, windows, cooling options, and interface. The Raman version is cooled to -40 °C (dry gas) detector using a CCD30-11 sensor from e2v, with a USB connector. All cameras are build to MilSpecs, meaning they are rugged and reliable to up to 75 °C. Other sensors as well as vacuum cooling options are available.
Renishaw	inVia Qontor	Confocal Raman microscope	Raman scattering	Provides continuous feedback to the sample stage, which adjusts to follow the height of the sample.
Technospex	uSight - X	Raman spectrometer	Raman scattering	Laser-induced fluorescence, photoluminescence, and Raman spectroscopy.
Thermo Fisher Scientific	DXR2	Raman microscope	Raman scattering	Submicrometer resolution images for chemical identification. Obtains morphological and structure information. Data interpretation is immediate and visually informative
WITec GmbH	alpha300 access	Raman microscope	Single spot analysis and imaging in reflection	A high-quality confocal micro-Raman system for analysis of the smallest sample volumes. It enables single-spot analysis or Raman mapping with exceptional spectral quality. For budget-conscious customers requiring high performance optical throughput and spectroscopic capabilities. Full upgradeability to 3D Raman imaging, AFM, and NSOM to keep pace with emerging and future challenges.

N/A = not applicable

Table IX: Software products

Company Name	Product Name	Product Type	Measurement Mode	Applications and Unique Features
ACD/Labs	ACD/ ChemAnalytical	ChemAnalytical workbook	N/A	Software that allows analytical data from different techniques, in different formats to be reviewed, analyzed, and interpreted in one interface. Stores live spectra with interpretations and related chemical structures.
ASD Inc., a PANalytical company	FieldSpec	Dual collection software	N/A	The world's first full-range (350–2500 nm) field solution that enables collection of high-quality spectra under variable sky conditions. Dual collection of white reference and target radiance measurements from two field spectrometers, minimizing the influence of atmospheric conditions.
Autoscribe Informatics	Matrix Gemini	Business information management system	N/A	Tracks assets, helpdesk issues, and actions. Manages staff competencies, controlled documents, customer feedback, and much more.
Bio-Rad Laboratories	KnowItAll Deformulation Expert	Software that suggests mixture formulations from spectra	N/A	Suggests the formulation of commercial products.
	KnowItAll QC Expert	Dedicated software for QC of chemical products	N/A	21 *CFR* Part 11-compliant software that performs a rapid check of an IR or Raman spectrum against a reference spectrum to verify that the material meets specifications. The software also compares the sample to a reference database to ensure that the sample does not match anything else in the database.
	KnowItAll Vibrational Spectroscopy Edition (IR)	Vibrational spectral analysis software for IR spectra	N/A	Offers comprehensive solutions for spectral analysis, identification, search, data management, and reporting. The software is intended to be combined with a spectral reference collection to help chemists extract information from their spectral data.
	KnowItAll Vibrational Spectroscopy Edition (Raman)	Vibrational spectral analysis software for Raman spectra	N/A	Same as for KnowItAll Vibrational Spectroscopy Edition (IR)
BioTools	Prota-3S Software	Software for PROTA-3S protein analyzer	N/A	Provides 1–2 min collection, low concentration (less than 0.25 mg/mL) capability, no limit on high concentration.
B&W Tek	BWID	Raman ID program	N/A	Provides rapid Raman spectroscopic identification and verification of materials. Designed for combination with the i-Raman series of spectrometers. Integrates spectral library and database capabilities with search and match algorithms. Includes library creation and one-click results. Users can save, view, and print customized analysis reports. Third-party libraries can also be used. Software is fully 21 *CFR* Part 11 compliant.
	BWIQ	Multivariate calibration software	N/A	For exploratory, qualitative, and quantitative analysis of spectral data. Combines traditional chemometric methods such as partial least squares regression and principal component analysis with support vector machine regression and classification algorithms for nonlinear datasets. Preprocessing tools include smoothing, normalization, derivatives, and adaptive iteratively reweighted penalized least squares algorithm for automatic baseline correction. The chemometrics software package can be used on-line with i-Raman Plus for real-time prediction.
	BWSpec Mobile	Operate and collect data using a touch-screen computer	N/A	Specifically designed for use on small touch-screen devices. Also allows users to collect and process data with the embedded touch-screen tablet computer on B&W Tek's mobile spectroscopy systems. Touch-screen software provides a simple graphical workflow. Users can control the device to collect data and can conduct real-time identification with spectral libraries and real-time predictions using chemometric models. Using this software, users can control the microscope attachment on the i-Raman Pro.

Table IX: Software products (continued)

Company Name	Product Name	Product Type	Measurement Mode	Applications and Unique Features
Fiveash Data Management	FDM ATR Drugs	Spectra of drugs and pharmaceuticals	ATR	ATR and FT-IR spectra of the entire FDM ATR Drugs spectral library were measured on a monolithic diamond ATR crystal. It includes almost all kinds of drugs: controlled substances, prescription, and over-the-counter pharmaceuticals and excipients.
	FDM ATR Drug Kit	ATR and FT-IR spectra of drug mixtures	ATR	An ATR and FT-IR spectral library models preselected mixtures of active ingredients, blended drugs, and drugs with excipients. More accurate results are obtained when searching drug mixtures with this library compared to neat compounds
Harrick Scientific	TempLink	FT-IR software	All FT-IR modes	Coordinates Harrick's temperature-controlled sampling accessories with FT-IR data acquisition. The user selects temperatures or time intervals to trigger data acquisition. This establishes an automated series of events.
Horiba Scientific	ICP Neo	Software for Horiba ICP-OES spectrometers	N/A	Has a new patented High Dynamic Range Detection (HDD) system mode, advanced QC protocols, and retrospective analysis. The interface offers a user-friendly GUI, and comes with tools, a proprietary ICP-dedicated wavelengths database, multiple user capability, log-off and log-on without stopping the sequence, user-defined windows, defined maintenance warnings, and diagnostics with real-time information.
John Wiley & Sons	Spectra Lab	Spectral database software	GC–MS, FT-IR, ATR-IR, Raman, UV–vis, C-NMR, H-NMR, Si-NMR, O-NMR	Provides researchers with access to 2.2 million MS, NMR, and IR spectra. This subscription-based spectral library features a combination of more than 175 spectral databases, in over 20 chemistry specialties, and over five instrument techniques, sourced from Wiley, Bio-Rad Sadtler, and others. This analytical platform supports GC–MS, FT-IR, Raman, ATR-IR, UV–vis, and X-NMR spectroscopy.
	Registry of Mass Spectral Data 11th Edition	Mass spectral database	N/A	The registry of over 775,500 mass spectra and 599,700 unique compounds provides researchers with assurance that their untargeted spectral search is the broadest available. Compatible with most manufacturers' systems including Agilent, NIST, PerkinElmer, Shimadzu, Thermo Fisher Scientific, and Waters.
Latitude Compliance Services	Train-Ready	Training management software	N/A	Allows for all types of training including read and understand, instructor-led, user-submitted, and competency-based training to ensure proficiency. Training can be developed in-house or purchased. Instrumentation training can be presented.
Metrohm	Vision Air	Data collection–analysis software	N/A	Modern, intuitive software for vis–NIR spectroscopic measurements offers two dedicated environments: routine and manager. For routine users, measurements are made as simple as possible, while managers or advanced users get full functionality and data access.
Spectral Sciences, Inc.	FLAMES	Hot gas and particle radiation model	N/A	FLAMES is a software model that calculates the spectrum of a multi-constituent hot gas along a line-of-sight with multiple hot and cold layers. It is used for interpretation of IR spectroscopic measurements, including imaging spectroscopy, verification of hot gas spectroscopic measurements, retrieval of gas components, and quantitative analysis.
Texas Instruments	TI DLP NIRscan	Nano Software v2.0	N/A	Builds on existing software with the implementation of slew scan capability and programmatic control of integration times. Programmable adjustments allow capture of more detailed and accurate data over target wavelength ranges.

N/A = not applicable

correction of varying sky conditions. Software from Autoscribe Informatics can track assets, help-desk issues, staff management, customer feedback, and other administrative tasks. B&W Tek's software, together with its Raman spectrometers, can integrate spectral library information with its search and match algorithms. Metrohm has developed intuitive software for vis–NIR spectroscopic measurements under two dedicated environments.

Spectral Libraries

Bio-Rad's new offering, together with the company's spectral libraries, can suggest formulations of mixtures. Fiveash has spectral libraries of controlled substances and also of prescription drugs and excipients. Spectral Sciences' software also can calculate the spectra of gas mixtures, thereby performing de facto analysis of the mixture. John Wiley provides spectral database software to access 2.2 million MS, NMR, and IR spectra.

Hardware Control

We don't generally review instrument control software, because such software has traditionally been a part of hardware development. However, this situation is changing, driven by software platform obsolescence and customer expectations for touch screens and cell-phone like features. This area should prove to be an interesting field of development as vendors redefine workflows, data collection, and data analysis through the lens of usability.

BioTools' software, in conjunction with the company's protein analyzer, can collect spectra in 1–2 min and measure concentrations as low as 0.25 mg/mL. Harrick Scientific's software coordinates temperature-controlled sampling accessories with FT-IR data acquisition. Texas Instruments has added new features that build on its existing software; these include slew-scan capability and programmable integration times, as well as other programmable adjustments.

Horiba provides a new patented high dynamic range detection (HDD) system mode, advanced quality control (QC) protocols, and retrospective analysis. Latitude Compliance Services' training management software allows for all types of training under its jurisdiction.

UV–vis

UV–vis Trends

The lines between different spectral regions is becoming blurred. About 50 years ago, all UV–vis instruments (Table X) were de facto touted as UV–vis–NIR, but the NIR performance was, to put it kindly, generally unsatisfactory by modern standards. The new generations of instruments are becoming competitive with modern NIR-only spectrometers. Technospex is showing a new instrument with coverage of UV, visible, and NIR ranges.

UV–vis, like Raman and NIR, is seeing smaller sizes—in both instruments (such as those launched by International Light Technologies, SpectroClick, and Industrial Test Systems) and sample sizes (for example, the product launched by Thermo Fisher Scientific). Like the other classes of instruments noted earlier, there is also development around specific analyzers. UV–vis has long been a static field, with minor tweaks around basic instruments; it is good to see the level of innovation and development of increasing power in stand-alone instruments bringing new vitality and purpose to these tools.

UV–vis Products

Mettler-Toledo has a completely new instrument line that is compliant with pharmacopeial regulations and requires only one drop of sample. Spectral Evolution has a portable spectroradiometer for the 280–1900 nm spectral range and has an internal photo-trigger. The company tec5USA has an on-board processor to analyze spectral data in real time. Technospex has a UV–vis–NIR instrument for reflection, transmission, and absorption measurement at the microscale. Thermo Fisher Scientific's instrument can analyze DNA, RNA, and protein samples with 1–2 μL of sample. The instrument from Carl Zeiss has long-term stability and does not need frequent external calibration; it can also operate in stand-off mode.

Commercial Smart-Phone-Based and Miniaturized Spectrometers

Industrial Test Systems has a photometer system that pairs directly with a smart-phone or tablet via two-way Bluetooth communication. International Light Technologies provides a handheld illuminance spectrometer for the 360–780 nm wavelength range. SpectroClick puts visible reflection and absorption spectrometry in the palm of the user's hand with a single universal serial bus (USB) cable; SpectroClick also has the only instruments shown at Pittcon designed specifically for marketing to the academic marketplace (also see PerkinElmer, however, in the mid-IR section).

The new Avantes spectrometer offers 10× higher speed USB 3.0 communication. B&W Tek provides a portable spectrometer reflectance probe covering UV, visible, and NIR spectral ranges (350–2500 nm). MilliporeSigma uses identification bar codes for method selection and simplified data acquisition. PerkinElmer provides a family of instruments with a variety of spectral bandwidths for materials testing, QC, or research and development (R&D) applications. StellarNet has a spectrometer with a concave holographic grating and no mirrors, thereby reducing stray light and aberrations.

See Table X for details about the companies and products for this section.

X-ray

We might think that all (or almost all) X-ray equipment (Table XI) for chemical analysis is based on X-ray fluorescence (XRF), but that's not the case. Apco makes a Mossbauer spectrometer, which is specially sensitive to iron (Fe) atoms. This is the basis for a specialized microscope for steel and other iron-containing materials.

Heuresis makes an XRF spectrometer that is a handheld device using ordinary AA batteries for power—another example of the trend discussed in our introduction. Panalytical produces an energy dispersive X-ray fluorescence (EDXRF) device to measure elements ranging from sodium to americium at 2 ppm levels. Rigaku makes a high-performance EDXRF system that uses a 60-kV, 12-W X-ray tube (not portable). Spectro Analytical makes portable and nonportable XRF systems (for bringing to the plant floor) and EDXRF systems (for greater precision and accuracy).

Accessories

Accessories (Table XII) are generally designed to simplify the laboratory workflow around a major instrument. Under this umbrella, we see specialty laboratory furniture (IonBench), reference materials (Inorganic Ventures), sample delivery (Spetec GmbH and Cetac), and sampling devices (Czitech, Harrick, and Glass Expansion) all attacking some workflow pain point. In some cases, companies offer a "solution" that is a combination, sometimes of two major tools (like TGA–IR or rheometry–Raman), but more commonly a combination of a major instrument with a sampling device or relatively minor auxiliary device, like an autosampler on an ICP-MS instrument. As should be expected, different accessory vendors often identify the same market needs, such as with diamond FT-IR ATR devices (at least seven different vendors). In addition, the trend noted earlier regarding low-cost instrumentation includes devices where the accessory becomes an essential part of a targeted solution.

Sample Preparation

In this vein, Anton Paar offers an improved sample digestion system that prepares multiple samples for analysis simultaneously. Similarly, Claisse provides a device for improved sample preparation that prepares multiple fusion disks for atomic adsoprtion (AA) analysis simultaneously. Distek's device has 10 stations for simultaneous sample preparation.

Table X: UV–vis products

Company Name	Product Name	Product Type	Measurement Mode	Applications and Unique Features
Avantes	Avantes EVO series	UV–vis spectrometer	N/A	10× higher speed USB 3.0 communication. Gigabit ethernet second communication port. Also offers a fast microprocessor and 50× more memory.
B&W Tek	i-Spec 25	Portable UV–vis–NIR spectrometer	Diffuse reflectance	A broadband portable spectrometer reflectance probe for measurements from 350 to 2500 nm. Contains Si, InGaAs, and extended InGaAs arrays for optimal sensitivity and dynamic range. iSpec 4 software provides control and data collection for multiple spectrometers.
Carl Zeiss Spectroscopy GmbH	Corona Process	UV–vis process spectrometer	Reflection	Provides long-term stability. Does not require frequent external calibration. Same accuracy at a distance of 80 to 600 mm from the sample, unaffected by temperatures from -10 °C to + 50 °C.
	Thin Process	Layer thickness and color analysis instrument	Reflection, transmission	Rapid layer thickness and color analysis. Efficient in situ process control. Coating uniformity.
Industrial Test Systems, Inc. (ITS)	eXact iDip	Smart photometer system	Transmission	Handheld photometer system with Bluetooth, pairs directly with a smartphone or tablet. Two-way wireless communication allows for instantaneous software updates and upgrades and customization.
International Light Technologies	ILT350	Illuminance spectrophotometer	Lux/fc and spectrum	Handheld, ergonomically designed, visible range (380–780 nm) illuminance spectrophotometer. Color screen, rechargeable battery, internal memory for sample scans and baseline, on-screen analysis. Internal software measures Lux/fc, Peak, CCT, CRI, dominant wavelength and Purity, XYZ, 2 and 100, RA, purity, and Delta UV.
Mettler-Toledo	Excellence	UV–vis spectrophotometers	Transmission	Completely new spectroscopic instrument line. Provides speedy and reliable measurements. Compliant with pharmacopeia regulations. Requires only one drop of sample over a wide concentration range.
Millipore Sigma	Spectroquant Prove 100, 300, and 600	UV–vis spectrometers	Transmission	Use live identification bar codes for method selection to simplify data acquisition and operation, and eliminate the need to rezero when switching between analytes. Lamps are guaranteed for life; users can recalibrate using calibration kits.
PerkinElmer	Lambda 265/365/465	UV–vis spectrometers	190–110 nm transmission and reflectance	A family of UV-vis instruments offering a variety of spectral bandwidths for materials testing, QA and QC, and R&D.
Spectral Evolution	SR-1901PT	Portable spectroradiometer	Reflectance, absorption	Spectral range is 280–1900 nm, features adjustable integration and scan averaging time, internal phototrigger with SMA-905 port, 0–100 ms trigger delay increment.
SpectroClick	AAH-300	Visible absorption and reflection spectrometer	Transmission or reflection	Designed for handheld visible reflection and absorption spectrometry. A single USB cable connects the light source, sample holders, dispersion, and detection, in a low power package, to a Windows laptop. Autocalibration corrects wavelengths. Resolution to 2 nm, with 10 nm at low light levels.
	SpectroClick Kit	UV–vis spectrometer teaching kit	Transmission	Intended for academic use: K–12 or college. The provided items can allow the user to build and manipulate a rudimentary spectrometer.
StellarNet	Black-Comet -TEC	UV–vis spectrometer	Transmission, absorbance, reflectance, color, radiometer, solar measurement	Designed to use holographic concave grating, which improves spectral shapes by reducing aberrations. Design uses no mirrors, thus reducing stray light.
	Blue-Wave	UV–vis spectrometer	Transmission, absorbance, reflectance, radiometer, color	Rugged and can function in the harshest conditions. Every component is fixed in place. Calibrations remain accurate no matter the environment. Modular nature; allows one instrument to be capable of multiple measurements.
	Solar-Rad	Research-grade spectrometer	Transmission, absorbance, reflectance, radiometry, solar monitoring	Radiometric measurements, modular system allows one spectrometer to couple with receptors (for solar measurements, integrating spheres for LED's and indoor lighting). Ranges from 200–100 nm to 200–1700 nm.
tec5USA	tecSaaS	UV–vis–NIR spectrometer	Transmission or reflection	On-board processor, processes spectral data in real time. Complex algorithms can be programmed into the electronics.

Table X: UV–vis products (continued)

Company Name	Product Name	Product Type	Measurement Mode	Applications and Unique Features
Technospex	uSight – 2000	UV–vis–NIR spectrometer	Reflection, transmission, absorption	UV–vis–NIR reflectance, transmittance, and absorbance measurement at microscopic levels. Can also be equipped with Raman, fluorescence, dark field, bright field, and polarization capability.
Thermo Fisher Scientific	NanoDrop One	Microvolume UV–vis spectrophotometer	Transmission	Analyzes DNA, RNA, and protein samples with only 1–2 μL of sample. High-resolution touchscreen interface, auto-range pathlength technology, accurate measurements of concentrated samples.

N/A = not applicable

Table XI: X-ray products (including gamma-ray and other higher-frequency methods)

Company Name	Product Name	Product Type	Measurement Mode	Applications and Unique Features
Apco Ltd.	Mössbauer Spectroscopic Microscope	Mössbauer spectroscopic microscope	Transmission, internal conversion electron, and so forth	MSM evaluates microstructure of Fe atoms in materials. Combines the MSM with a scanning electron microscope (SEM), an electron beam induced current (EBIC), an electron backscatter diffraction (EBSD), and an electron energy analyzer. A multicapillary X-ray lens achieves a spatial resolution of several micrometers.
Heuresis Corporation	Pb200i	Lead paint analyzer	X-ray fluorescence	Android-based handheld XRF instrument. Includes built-in WiFi, Bluetooth, GPS, and a color camera. Uses rechargeable or disposable AA batteries. Can store up to 65,000 readings, including spectra and photo of the sample.
PANalytical	Epsilon 3XLE	EDXRF chlorine-in-crude XRF system	EDXRF	Measures chlorine in crude oil at 2 ppm levels in the presence of percentage levels of sulfur. Can compensate for variable characteristics of crude oil composition. Can analyze all other relevant elements from sodium to americium with similar accuracy and repeatability.
Rigaku Corporation	Nex DE VS	High-performance, variable small spot EDXRF elemental analyzer	N/A	A high-performance, direct excitation EDXRF elemental analyzer. Contains a 60-kV, 12-W X-ray tube, high-throughput Si drift detector, collimators, high-resolution camera. The Si drift detector has count rates of over 500 K cps for low LOD.
Spectro Analytical Instruments	Spectroscout	X-ray fluorescence spectrometer	EDXRF	Portable analyzer eliminates time spent transporting samples from the plant floor to the laboratory. Surpasses other portables at half the cost of a dedicated laboratory instrument.
	Spectro Xepos ED	EDXRF spectrometers	EDXRF	Multielemental analysis of major, minor, and trace element concentrations, new developments in excitation and detection, gains in precision and accuracy, faster measurements. Redesigned operating software quickly and accurately analyzes practically any unknown liquid, powder, or solid sample.

N/A = not applicable

Instrument Add-Ons

Biotools has a temperature controller for sample cells, which will result in improved spectral consistency. Stellarnet also provides temperature controllers. Czitek offers an adapter to couple microscopy optics to a FT-IR spectrometer, as well as a video attachment for ATR spectroscopy. Glass Expansion provides several accessories to improve the performance of various atomic spectroscopic techniques. For molecular spectroscopy, Harrick and Hellma-Axiom have improved diamond ATR add-ons. Specac has a sample holder for viscous samples. IonBench has a positioner for putting a high performance liquid chromatography (HPLC) column near the inlet of a mass spectrometer. Spetec has a syringe pump to measure reproducible amounts of sample. Teledyne-CETAC also provides a syringe pump.

External Control

MS Noise offers soundproofing for noisy lab equipment. Ocean Optics has an improved substrate for surface-enhanced Raman spectroscopy (SERS). Quantum Composers provides advanced control of lasers for Raman, for example.

Combining Instruments

Headwall Photonics offers a data-acquisition system that fuses data from different technologies. Ondax offers a similar capability in coupling low-frequency Raman with chemical fingerprinting. Xia offers an eight-channel pulse processor for high-resolution X-ray spectroscopy.

Table XII: Accessories

Company Name	Product Name	Product Type	Measurement Mode	Applications and Unique Features
Anton Paar	Multiwave GO	Microwave digestion system	N/A	Fast, simple, and affordable microwave digestion system. Digests 12 samples in as little as 18 min.
BioTools	TempCon-2X	Temperature controller	N/A	Peltier-based temperature controller for use in FT-IR spectrometers. Two types of windows: circular BioCell windows and hexagonal windows. Manual or computer control. Interface can be aligned with FT-IR scanning software.
Claisse	TheOx Advanced	Fusion instrument	N/A	Prepares glass disks for XRF analysis as well as borate and peroxide solutions for ICP and AA analysis. Has six fusion positions, is fully automatic, and can fuse 24–30 samples per hour.
Czitek	MicromATR Vision	Combined imaging and ATR	ATR	Sample compartment accessory for FT-IR that combines ATR with video imaging.
	SurveyIR	Microspectrometer	Transmission, reflection, and diamond-ATR	Couples integrated digital video microscopy with IR microspectroscopy in a compact package that mounts in the sample of a standard FT-IR instrument.
Distek, Inc.	PrepEngine	Prepare content uniformity samples	N/A	A 10-station system that can prepare content uniformity samples to speed up the sample preparation process: up to 90% faster than traditional methods. Adjustable speeds range from 500 to 6000 rpm and run times from 5 s to 30 min.
GFS Chemicals, Inc.	IN SPEC	UV–vis validation kit #87020	Absorption or transmission	Inert, NIST traceable, and inexpensive reference materials are an easy way to verify a UV–vis spectrophotometer's photometric accuracy, wavelength scale, and stray light.
Glass Expansion	DC Nebulizer	Nebulizer	ICP-OES, ICP-MS	Combines the benefits of the U-Series nebulizer with a direct-connect argon line to ensure a leak-free gas connection.
	D-Torch	Demountable torch	ICP	Offers interchangeable quartz and ceramic outer tubes and interchangeable injectors.
	Elegra	Argon humidifier	ICP	Uses highly efficient membrane technology to add moisture to the argon. Inert metal-free construction. Requires no heating or electric power.
	IsoMist XR	Temperature controller	ICP	Controls and monitors the ICP spray chamber temperature over a range of -25 °C to +80 °C. Temperature held within +/- 0.1 °C.
Harrick Scientific	DiaMaxATR	Diamond ATR	ATR	New single-reflection diamond ATR designed for high optical throughput throughout the mid-IR. Monolithic diamond ATR element enables simplified analysis of a wide range of sample types, including hard solids, abrasive powders, and corrosive liquids.
Headwall Photonics	HyperCore	Data acquisition system	N/A	A data-acquisition system that provides sensor fusion among commonly used instruments. 500 GB internal drive, 2 GB-E ports, GPS connection, base camera link.
Hellma Axiom Inc.	DMD-373	Diamond ATR probe	ATR	A unique combination of high transmission and small diameter. The extreme chemical resistance provided by the diamond ATR element and Hastelloy construction makes it suitable for mid-IR process monitoring without requiring a cooled IR detector.
	DPR-212	High transmission ATR probe	ATR	A straight mid-IR ATR probe that features a transmission of over 20%. The high transmission and straight configuration make it especially appropriate for small FT-IR spectrometers such as the Bruker Alpha and Thermo iS5 and iS10.
Inorganic Ventures	CGNB2O51 and CGNB2O510	Ta free niobium standard for ICP	N/A	A certified reference material set in a nitric acid matrix traceable to NIST, ISO 17025, and ISO Guide 34. Packaged in TCT bag, which extends the life of the product.
	CGZRCL10	Zirconium standard in HCl for ICP	N/A	Same as Ta free niobium.
	IV-STOCK-60	USP 232 drug substance and excipients standard	N/A	Same as Ta free niobium.
	TUNE F-X-SERIES	Certified reference material set in a nitric acid matrix for stability	N/A	Same as Ta free niobium.

Table XII: Accessories (continued)

Company Name	Product Name	Product Type	Measurement Mode	Applications and Unique Features
IonBench	IonBench	LC elevator bench for HPLC	N/A	Simplifies the orientation of the HPLC column to ionization sources. Operators can safely lower it to a desired height, then precisely return to its operating height.
	IonBench for Waters Vion IMS QTof	LC elevator bench for Waters Vion IMS QTof	N/A	Accepts a weight load of 400 kg (1010 lb), delivers significant space savings and 75% noise reduction from the vacuum pump. Serves as waste reservoir, provides soundproof enclosure with 15-dBA sound suppression, overheat alarm.
MS Noise	DBL-OM	Acoustic enclosure	N/A	Soundproofs vacuum pumps to suppression of 15 dBA, using soundproofing materials such as ABS and 2-in. of heat-, oil-, and flame-proof insulation material.
Ocean Optics	Nanosponge	SERS substrate	Raman	Comprises a porous gold–silver alloy film on a glass substrate, which makes it usable with 532-, 638-, and 785-nm laser excitation. Optimum at 638-nm excitation.
Ondax	TR Probe	Terahertz–Raman spectroscopy probe	Raman scattering	Simultaneously captures low-frequency and chemical fingerprint signals, for both chemical composition and molecular structural analysis in a single measurement. Low-frequency Raman probe designed for in situ process monitoring, in-line testing, bulk, or sample testing applications.
Quantum Composers Inc.	Smart Controller	Laser controller	N/A	Smart controller for our LS-625 and LS-635 laser systems. Can be used with manual systems where a microscope is needed to manually repair wafers, dies, and other applications.
Specac	Pearl	Liquid transmission analysis accessory	N/A	Offers a highly repeatable pathlength for viscous or runny samples. Samples are introduced via pipette or syringe. Wedged Oyster Cell prevents fringing patterns. Pathlength is changed by replacing the lower window of the sample tray.
Spetec GmbH	Symax	Syringe pump	N/A	Meters fluids in micro or nanoliter quantities using a stepper motor drive connected directly to the drive spindle, reducing mechanical play. The delivery range lies between 0.5 nL/min and 44 mL/min.
Starna Cells	Starna FTIR Polystyrene Wavelength Reference Material	Polystyrene wavelength reference material	Transmission	Manufactured and certified to ISO Guide 34 and ISO/IEC 17025 accreditations.
	Starna USP <857> UV Qualification Kit	UV standards	Transmission	Fully heat-fused sealed certified reference materials, manufactured and certified under ISO Guide 34 and ISO/IEC 17025 accreditations.
	Demountable Cell	Demountable microvolume DMV-Bio Cell	N/A	Patented low-volume demountable cell, enabling validated, reliable, and reproduce analysis of microvolume samples of any highly concentrated materials on virtually any standard spectrophotometer. Extends the capability of standard spectrophotometers.
StellarNet	2-Stage Thermo Electric Cooler	Add-on thermoelectric cooler	N/A	Reduces the temperature to 30° below ambient, increasing instrument S/N by 80% and improving low light measurement quality for Raman, fluorescence, and other weak light emission applications. Improves the stability of the detector for lengthy measurements where thermal noise disrupts the signal.
Teledyne CETAC Technologies	SDXHPLD	High-performance liquid dilution system	N/A	Combines the company's ASX-560 autosampler with a novel vortex mixing dilution accessory. Makes use of a high-precision syringe pump for both aliquot and diluent,
Xia LLC	FalconX8	Multichannel pulse processor for X-rays	N/A	An eight-channel digital pulse processor for very high rate and high resolution X-ray spectroscopy. The processing dead-time has been reduced from 70% to just a few percent, maintaining energy resolution, thereby maximizing data collection efficiency and reducing run times at synchrotron beamlines and in other high-rate applications.
	Pixie-4e	Multichannel pulse processor for gamma ray spectroscopy	N/A	A four-channel digital pulse processor for high-resolution gamma spectroscopy, timing spectroscopy, and waveform analysis with most detector types, including HPGe detectors and scintillators. Processor speed options range from 125 to 500 MSPS. Coincidence gating between channels and a real-time on-board pulse shape discrimination, to separate neutrons from gammas in scintillator detectors. The PXI Express platform permits data transfer rates over 400 MB/s.

N/A = not applicable

Table XIII: Components

Company Name	Product Name	Product Type	Measurement Mode	Applications and Unique Features
BaySpec	OEM	UV–vis–NIR, Raman spectrographs and spectrometers	N/A	Fully customized spectroscopic systems for resolution, optical throughput, input configurations, and footprint design.
Clippard Instruments	NIV Series	PTFE media isolation valves	N/A	One-piece valve stem that functions as a sealing membrane.
Cobolt	Cobolt DPL 532 nm	Diode-pumped solid state laser (DPSSL)	N/A	Single longitudinal mode (SLM) DPSSL. Now available with an integrated optical isolator for analysis of highly reflective samples. Has up to 160 mW after the optical isolator, and has excellent spectral purity and wavelength stability.
	Cobolt NLD 785 nm	Tunable optical parametric analyzer	N/A	Frequency-stabilized diode laser at 785 nm. Has up to 500 mW output including an integrated optical isolator. Totally integrated electronics, can be incorporated into high-end Raman based systems.
	Cobolt Odin	Narrow linewidth, tunable mid-IR source	N/A	Based on a fully contained, temperature tunable, optical parametric oscillator (OPO) and integrated pump laser. Periodically poled nonlinear optical crystals are used, mid-IR emission from 2 to 5 µm, at 10 kHz, with <5 ns pulse widths.
Crystal IS	Optan Flat Window	Deep UV LEDs	N/A	Offer better stability of light, higher light intensity, and lower power consumption than deuterium lamps. Provides lower limits of detection and reduced detector cost. Are based on native aluminum nitride (AlN) substrates and are designed to overcome limitations of other LEDs and provide higher light output, providing better reliability and allowing electronics to be isolated from flow cells.
	Optan SMD	Deep UV LEDs	N/A	Compact footprint allows for design flexibility and integration into instruments of all sizes while providing industry-leading light output and reliability for instrumentation applications. UVC LEDs can prevent biofilm formation, counteracting the impact of this severe problem.
Headwall Photonic	High-performance Holographic Diffraction Gratings	Diffraction gratings	N/A	Headwall's master-quality gratings are available in planar, concave, and convex designs. Attributes are exceptionally small sizes, temperature insensitivity, low stray light, high S/N, and aberration correction for high spectral and spatial resolution.
Inrad Optics	X-ray monochromator	X-ray monochromator	N/A	Focuses an X-ray source to a small spot. High intensity for X-ray photoelectron spectroscopy (XPS). Quartz, germanium, and silicon crystals are polished and oriented to within 20 arc-seconds of their 2D crystal plane spacings. Applications: elemental surface analysis, plasma diagnostics, laser induced X-ray sources.
Microcertec	3D Interconnect Circuit	3D interconnect circuit on ceramic carrier	N/A	Enables customized packaging solutions with more flexibility than photolithography techniques for 2D and flat surfaces. This new type of component combines precision-grinding of ceramics with thin-film metallizing and laser micromachining.
OptiGrate Corp.	BragGrate	Notch filters	N/A	Enable measurements of Raman bands down to 4 cm^{-1} with a single stage monochromator. They also have broad transmission region that covers the complete frequency range of ±4000 cm^{-1}.
Polymer Char	IR5 MCT	Infrared detector	N/A	Mercury-cadmium-telluride infrared detector designed to determine on-line concentration and short-chain branching in polyolefins. Provides sensitivity and long-term baseline stability.
QMC Instruments	Cryogen-free THz Bolometer	Terahertz detector	Transmission, reflection	Superconducting bolometer offers high sensitivity without liquid helium. Push-button operation. Can operate continuously for months. Only electricity is needed. Can be configured for frequencies up to 2000 cm^{-1}. Provides a linear dynamic range of greater than 70 dB.
Quantum Composers Inc.	Micro Jewel	DPSS lasers	N/A	Rugged, Q-switched, Nd:YAG, DPSS lasers have a compact, monolithic design. Reliable, lightweight, with easy-to-swap components. Designed for commercial and OEM applications.
	MIR	Mid-IR lasers	N/A	Factory-selectable output pulse energies in a compact and robust package. Diode pumped, no need for scheduled maintenance or water cooling. Can be integrated into laboratory experiments, or used as OEM unit.

Standards

To aid in obtaining accurate analyses, NIST-traceable standard samples are provided by GFS Chemicals. Inorganic Ventures also provides several different sets of certified reference materials (CRMs). Starna Cells provides wavelength standards for IR and UV spectroscopy.

Components

As we noted above, in our taxonomy *components* (Table XIII) are devices that are used in the construction of an instrument or items that become inherently part of an instrument—if the component is absent, the instrument does not work or becomes severely degraded. As an example, all modern Raman instruments need a laser and an optical filter, among other things. Without the laser, there is no signal and without the filter, the laser illumination will overwhelm the detector. This type of device is different from an accessory that can be used optionally in conjunction with an instrument and is generally external to it; the instrument will work just fine without it, but the accessory extends the instrument's capabilities (for example, a liquid flow cell for an instrument innately designed to measure solid samples).

Easily, the most numerous component announcements involve lasers, with at least five vendors announcing new or revised laser offerings this year. These offerings provide new wavelengths, new packaging, and higher powers for many applications. The array of lasers is opening new analytical areas with specificity not seen previously. Most of these lasers are now solid-state lasers (SSLs) in small packages, helping drive the handheld device market, especially for Raman spectroscopy. The grating vendors and optical filter manufacturers are responding with complementary tools (such as Headwall, Ocean Optics, and OptiGrate) to complete the packaging.

As the market continues to drive toward lower costs and smaller footprints, these tools will be the building blocks for the next generation of devices. With their increasing reliability and better performance, the lasers will begin to show up in more laboratory equipment as well.

One very interesting development is a cryogen-free bolometer from QMC Instruments. This component could enable more laboratories to explore the long-wavelength IR (terahertz) region of the spectrum with a high sensitivity detector. Further developments in this space will be worth watching.

Bayspec is offering modular spectrometric "building blocks" for UV, visible, and NIR measurements for OEMs. Texas Instruments has spectrometer modules based on its TI DLP technology. Clippard Instruments has one-piece PTFE valves for sample handling. Tornado Spectral Systems has a virtual slit that increases the spectral throughput of a Raman spectrometer.

Lasers and Sources

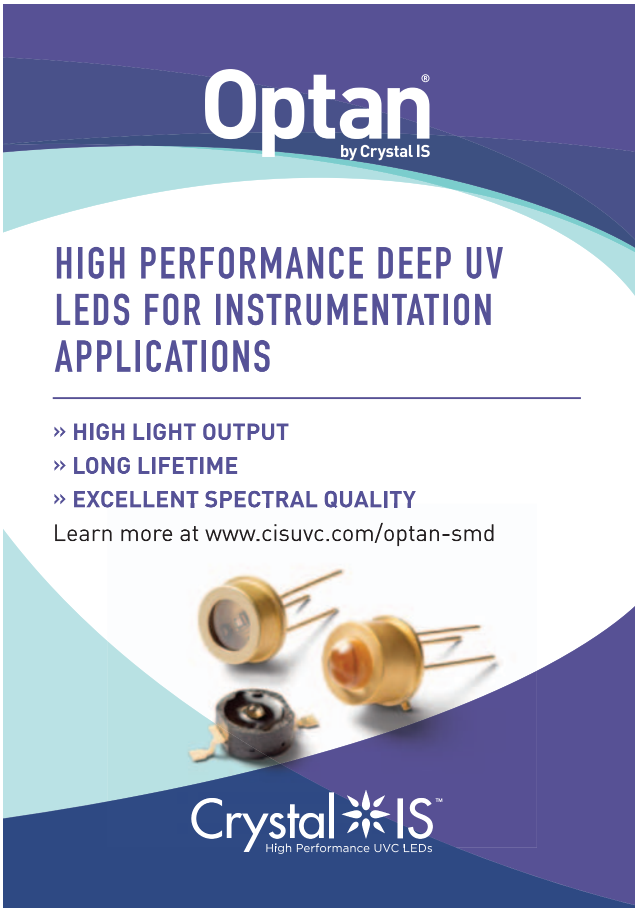
Adding to the laser list above, Cobolt provides a single-longitudinal-mode SSL with integrated optical isolator, as well as

Table XIII: Components (continued)

Company Name	Product Name	Product Type	Measurement Mode	Applications and Unique Features
RPMC Lasers Inc.	Oxxius	266 nm–280 nm deep UV CW laser	N/A	The most compact cw deep UV source on the market. Proprietary monolithic cavities technology is inherently stable and robust to vibrations.
	LCX	Laser module at 532, 553, and 561 nm	N/A	The next generation of monolithic DPSS lasers at 532, 533, and 561 nm. The LCX series is the most powerful, compact and efficient laser of its category.
	Quantas	1–10 Hz lasers	N/A	1053-nm or 1064-nm lasers. Up to 70 mJ at 1053 nm and up to 50 mJ at 1064 nm.
Spellman High Voltage Electronics Corp.	MX10plus	10-kV power supply	N/A	RoHS compliant MX10 is a well-regulated, high performance dynode power supply. 25 ms “hot switchable” polarity reversing capability.
Texas Instruments	3rd Party and OEM Spectrometer Modules based on TI DLP	Pspec-NIR from QEA	Transmission, reflection	Battery-powered stand-alone solution. Lightweight, compact, and portable, versatile and cost-competitive configurable platform.
Tornado Spectral Systems	HyperFlux PRO Plus	High-throughput virtual slit	N/A	Enhances the spectral throughput of Raman spectrometers by an order of magnitude over conventional designs. Process measurements can be done faster, with better sensitivity. Preserves samples through the use of lower laser powers.

N/A = not applicable

tunable parametric oscillators for various wavelength ranges. Quantum Composers provides an SSL for various wavelength ranges. RPMC Lasers provides a laser for deep-UV operation as well as for more conventional wavelength ranges. An alternative to lasers is LEDs, which come in various wavelength ranges. Crystal IS offers deep-UV LEDs in various configurations.



Wavelength Selection

Other components for spectrometers include wavelength-separating components, such as Headwall Photonics’ holographic diffraction gratings and Inrad Optics’ X-ray monochromator. Optigrate has a different approach with narrow notch filters to remove the laser line in Raman spectroscopy.

Electronics

Every instrument needs electronics. Microcertec has a way to reduce the space the electronics requires by using 3D packaging for them. Spellman High Voltage Electronics Corp. manufactures restriction of hazardous substances (RoHS)-compliant power supplies. Every instrument also needs a detector. Polymer Char has a mercury-cadmium-telluride (MCT) detector optimized for an instrument determining chain length and branching in polymers. As mentioned above, QMC Instruments has a superconducting bolometer that does not require liquid helium.

Howard Mark serves on the Editorial Advisory Board of *Spectroscopy* and is a regular coauthor of the “Chemometrics in Spectroscopy” column. He also runs a consulting service, Mark Electronics, in Suffern, New York. **Mike Bradley** also serves on the Editorial Advisory Board of *Spectroscopy* and is a marketing manager for FT-IR and FT-IR microscopes at Thermo Fisher Scientific in Madison, Wisconsin. Direct correspondence to: hlmark@nearinfrared.com ■

For more information on this topic, please visit our homepage at: www.spectroscopyonline.com

PRODUCTS & RESOURCES

FT-NIR analyzer

The TALYS ASP400 single-point fiber optics–based industrial FT-NIR analyzer from ABB is designed for real-time monitoring of refinery and petrochemical process streams. According to the company, the on-line analyzer allows determination of stream qualities or physical properties, process characterization, and early troubleshooting. **ABB Measurement & Analytics,** Quebec, Qc, Canada; www.abb.com/analytical

EDXRF analyzer

Applied Rigaku's NEX DE VS direct-excitation, variable-spot X-ray fluorescence elemental analyzer is designed with a 60-kV, 12-W X-ray tube and a high-throughput Si drift detector. According to the company, the analyzer is suitable for applications such as research, bulk RoHS inspection, education, and industrial and production monitoring. **Applied Rigaku Technologies, Inc.,** Austin, TX; www.rigaku.com

NIR spectrometer

The AvaSpec-NIR512-2.5-HSC near-infrared spectrometer from Avantes is designed for measurements at wavelengths up to 2500 nm where higher resolution or more data points for multivariate modeling are required. According to the company, the spectrometer has double the amount of pixels compared to its NIR256-2.5-HSC model. **Avantes, Inc.,** Bloomfield, CO; www.avantes.com

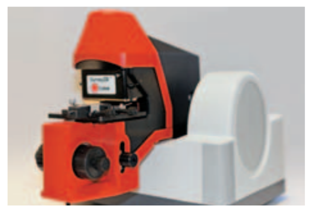
FT-NIR spectrometer

The TANGO FT-NIR spectrometer from Bruker is designed to enable high sample throughput and simultaneous evaluation of different components in food, feed, chemical, and pharmaceutical applications. According to the company, no sample preparation is required and the sample is filled into the measuring cup or vial with the measurement being done through glass. **Bruker Corporation,** Billerica, MA; www.bruker.com

Light sources

Optan surface-mounted-device light-emitting diodes from Crystal IS are designed as alternatives for UV lamps used in fluorescence spectroscopy, imaging, and biofouling control. According to the company, the light outputs range from 2 to 8 mW. **Crystal IS,** Green Island, NY; www.cisuvc.com

FT-IR microanalysis accessory



The SurveyIR FT-IR microanalysis accessory from Czitek is designed for microanalysis and image documentation of fibers, paints, polymers, fabrics, pharmaceutical active ingredients, excipients, narcotics, explosives, surface defects, paper contaminants, and minerals. According to the company, the accessory mounts in an FT-IR spectrometer's sample compartment and uses the spectrometer's detector. The accessory reportedly couples integrated digital video microscopy with IR microspectroscopy in a user-installed compact package. **Czitek,** Danbury CT; www.czitek.com

ICP nebulizer

Glass Expansion's DC nebulizer is designed with an instrument-specific direct-connect argon line. According to the company, the DC fitting eliminates the need for various adapters and extra tubing ordinarily required for connecting the nebulizer to the ICP gas port, and the nebulizer's metal-free container eliminates any potential for metal contamination. **Glass Expansion, Inc.,** Pocasset, MA; www.geicp.com

ATR accessory for FT-IR

Harrick's DiaMaxATR single-reflection diamond attenuated total reflectance accessory is designed to enable simplified analysis of a range of sample types, including hard solids, abrasive powders, and corrosive liquids. According to the company, available options include far-IR extended sampling, a digital force sensor, and heated flow cells. **Harrick Scientific Products, Inc.,** Pleasantville, NY; www.harricksci.com

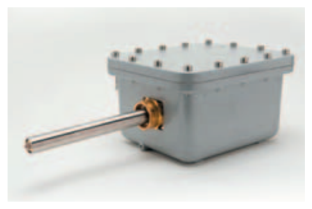
Custom certified reference materials

Inorganic Ventures' custom certified reference materials shipped in packaging that reportedly enables the standards to be stored for up to three years without compromising accuracy. According to the company, the one-year expiration date of the custom standard does not start until the Transpiration Control Technology packaging is opened.

Inorganic Ventures,
Christiansburg, VA;
www.inorganicventures.com

FT-IR spectrometer

Keit's microFTS FT-IR spectrometer is designed to be compact, rugged, and vibration-proof. According to the company, the spectrometer inserts directly into production equipment, eliminating the need for fiber-optic cables, remote sampling, and frequent recalibration, and enabling real-time reaction monitoring on production floors.



Keit Spectrometers,
Oxfordshire, UK;
www.keit.co.uk

NMR spectrometer

Magritek's Spinsolve benchtop NMR spectrometer is designed with a 60-MHz Halbach magnet. According to the company, the compact spectrometers are initially available for the nuclei combinations of proton and fluorine or proton, fluorine, and carbon, with phosphorus and other nuclei soon to be added.

Magritek,
Wellington, New Zealand;
www.magritek.com

Raman analyzer

Metrohm's Mira Raman analyzer is designed for instant analysis of complex samples, both liquid and solid. According to the company, two measuring modes are available: point-and-shoot, for direct, noncontact analysis in the container; and integrated vial mode, for secure sample insertion.

Metrohm USA,
Riverview, FL;
www.metrohmusa.com

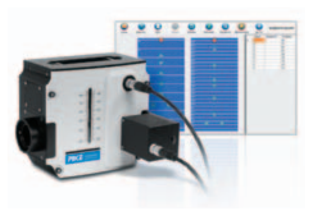
SERS substrates

Surface-enhanced Raman spectroscopy (SERS) substrates from Ocean Optics are designed for use in the detection of explosives and narcotics, food safety, anti-counterfeit tagging, and biological research. According to the company, its SERS substrates can amplify very weak Raman signals by many orders of magnitude for trace-level detection.

Ocean Optics,
Dunedin, FL;
www.oceanoptics.com

ATR sampling accessory

PIKE's updated Automated VeeMAX III variable angle specular reflection and attenuated total reflectance sampling accessory is designed with a motorized control for automated angle of incidence setting. According to the company, motor control and data collection are performed via AutoPRO6 PC software, which interfaces with most FT-IR software.



PIKE Technologies,
Madison, WI;
www.piketech.com

Terahertz detector

QMC Instruments' cryogen-free THz detector is designed with a closed-cycle electrically powered cooling platform. According to the company, the detector has a linear dynamic range of greater than 70 dB and provides an absolute measure of absorbed terahertz power down to picowatt levels.

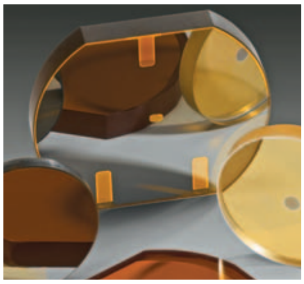
QMC Instruments Ltd.,
Cardiff, UK;
www.terahertz.co.uk

ICP-MS system

Shimadzu's ICPMS-2030 inductively coupled plasma–mass spectrometry system is designed for environmental testing, food and agriculture studies, and pharmaceutical work. According to the company, the system includes assistant functions that develop methods and perform post-run diagnostics.

Shimadzu Scientific Instruments,
Columbia, MD;
www.ssi.shimadzu.com

Infrared beamsplitters



Photon Pro infrared beamsplitters from Spectral Systems are designed for use in the analysis of hazardous materials, environmental control, process control, and material recognition on the manufacturing floor. According to the company, the beamsplitters simultaneously transmit and reflect 50% of the incident beam between two optical elements. **Spectral Systems LLC,** Hopewell Junction, NY; www.spectral-systems.com

NIR neutral density filters

NIR Metal-on-Quartz neutral density filters from Starna are certified reference materials designed to enhance and extend the capability to qualify the full range of transmittance scale of a UV-vis-NIR spectrophotometer. According to the company, the filters are protected from oxidation, physical degradation, or contamination by a novel cover plate that is optically bonded to the surface. **Starna Cells, Inc.,** Atascadero CA; www.starnacells.com

Thermoelectric spectrometer cooler

StellarNet's eXtreme thermoelectric detector cooler is available as an option for its Raman and SILVER-Nova spectrometers and is designed to lower the temperature of the charge-coupled device to 30 °C below ambient and increase instrument signal-to-noise ratio by reducing noise over 80% at long exposures. According to the company, the cooler includes a sealed and isolated detector enclosure with specialized heat sink and airflow design for added stability and cool operation. **StellarNet, Inc.,** Tampa, FL; www.StellarNet.us

Microspectroscopy system

TechnoSpex's uSight dual micro-spectroscopy system is designed to provide UV-vis-NIR and laser-induced spectroscopy functionalities such as Raman, photoluminescence, and fluorescence at levels down to a spatial resolution of less than 1 µm. According to the company, the system can be coupled with dark field, bright-field, and polarization for multimodality imaging. **TechnoSpex Pte Ltd,** Singapore; www.technospex.com

Understanding Single-Particle ICP-MS in Nanotoxicology and Ecotoxicology

ON-DEMAND WEBCAST | Originally aired April 20, 2016

Register for free at www.spectroscopyonline.com/spec/understanding

In this webinar, researchers from the SmartState Center for Environmental Nanoscience and Risk at the University of South Carolina will discuss the importance of measuring nanoparticle dose, concentration and transformations in order to understand nanotoxicology and ecotoxicology, including environmental fate and behavior. The discussion will have relevance for any process needing to measure nanoparticle concentration in any complex media. This will be followed by specific examples of how single-particle-ICP-MS has been used and developed at the center. These topics will include:

- Measuring the transformations of nanoparticles in media at environmentally relevant concentrations.
- Using single-particle -ICP-MS in conjunction with a separation device (FFF).
- Measuring exposure, dose, and uptake of ionic and particulate gold into phytoplankton.

Within each topic, a description of the experimental design will be discussed, highlighting the potential problems along with some results showing the importance of incorporating this technique into nanoparticle research.

Key Learning Objectives:

- Insights into environmental nanohealth issues — important factors in appropriate experimental design
- Application of state-of-the-art techniques related to nanometrology in environmental media (moderately hard water, algae, and daphnia media)
- Overview of method design related to toxicological and environmental studies — potential pitfalls

Who Should Attend:

- Environmental researchers
- Government regulators and researchers
- Toxicologists
- Academics

Presenters

Professor Jamie Lead
Endowed Professor and Director, SmartState Centre for Environmental Nanoscience and Risk, University of South Carolina

Ruth Merrifield
Research Assistant Professor, SmartState Centre for Environmental Nanoscience and Risk, University of South Carolina

Chady Stephan, PhD
Manager, Global Applications, Nanotechnology
PerkinElmer, Inc.

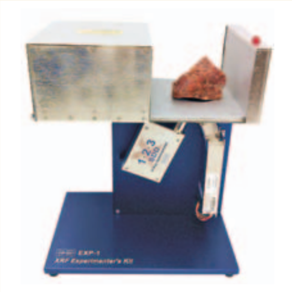
Moderator:
Laura Bush
Editorial Director
Spectroscopy

Sponsored by PerkinElmer For the Better

Presented by Spectroscopy

For questions, contact Kristen Moore at kmoore@advanstar.com

XRF kit



Amptek's XRF kit is designed to help users perform elemental analysis via X-ray fluorescence (XRF). According to the company, the kit includes the company's X-123 complete spectrometer with FAST SDD, SDD, or Si-PIN detector; mini-X USB-controlled X-ray tube; XRF-FP QA software; sample enclosure; and test sample.

Amptek Inc.,
Bedford, MA;
www.amptek.com

Modular spectrograph

The Shamrock 193i research-grade modular spectrograph from Andor is designed with a 193-mm focal length and is motorized. According to the company, the spectrograph is suitable for UV–NIR low-light fluorescence, Raman (SERS, CARS, and TERS), microspectroscopy applications, and routine spectral acquisitions.

Andor Technology,
Belfast, UK;
www.andor.com/spectroscopy/microspectroscopy

Carbon and sulfur analyzer

The EMIA-Pro carbon and sulfur analyzer from HORIBA Scientific is designed with measurement capabilities that range from 1.6 ppm to 6.0% for carbon, and 2.0 ppm to 1.0% for sulfur. According to the company, the analyzers can be used for a variety of inorganic materials such as steel, cokes, catalysts, non-ferrous alloys such as aluminum, and lithium-ion battery materials.

HORIBA Scientific,
Edison, NJ;
www.horiba.com/EMIA-PRO

Raman analyzer

The RamanRXN2 Multichannel analyzer from Kaiser is designed to provide high-resolution, research-grade Raman spectra on a portable platform for process development monitoring and control. According to the company, a single analyzer can collect Raman data from four channels, addressable by fiber-optic probes capable of direct in situ liquid or solid measurements in applications ranging from from raw materials identification to process control in a manufacturing environment.

Kaiser Optical Systems, Inc.,
Ann Arbor, MI;
www.kosi.com

ICP-MS system

Agilent's 7800 quadrupole ICP-MS system is designed for routine elemental analysis. According to the company, the system provides a wide dynamic range, matrix tolerance, and interference removal and includes software for method optimization and documentation.

Agilent Technologies,
Santa Clara, CA;
www.agilent.com

X-ray source

Moxtek's 12 W 60 kV X-ray source is designed for use with high-end benchtop XRF and XRD instruments. According to the company, the source's high accelerating voltage leads to improved analysis of elements with atomic numbers ranging from 47 to 60.

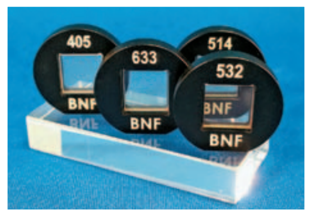
Moxtek Inc.,
Orem, UT;
www.moxtek.com

Terahertz Raman modules

Terahertz Raman spectroscopy modules from Ondax are designed to simultaneously capture low-frequency and chemical fingerprint signals. According to the company, the TR-Probe and TR-Bench modules deliver both chemical composition and molecular structural analysis in a single measurement for any process or laboratory environment.

Ondax, Inc.,
Monrovia, CA;
www.ondax.com

ULF Raman filters



BragGrate Raman filters from OptiGrate are designed to enable access to Stokes and anti-Stokes Raman bands in the ultralow terahertz frequency range down to 5 cm^{-1}. According to the company, laser line cleaning and light rejection notch filters are provided, and the filter production line is extended to cover many standard and custom laser wavelengths from 405 nm to 1550 nm.

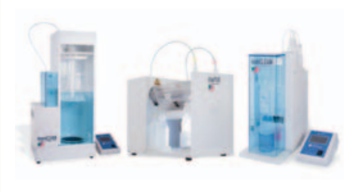
OptiGrate,
Oviedo, FL;
www.optigrate.com

Confocal Raman microscope

Renishaw's inVia Qontor Raman microscope is designed with LiveTrack, which reportedly enables users to analyze samples with uneven, curved, or rough surfaces. According to the company, optimum focus is maintained in real time during spectral acquisitions and white light imaging, eliminating the need for manual focusing, prescanning, or extensive sample preparation.

Renishaw,
Hoffman Estates, IL;
www.renishaw.com/Raman

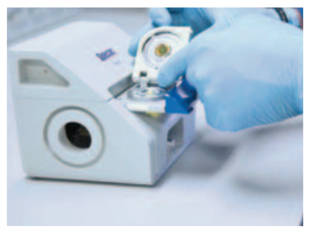
Atomic spectroscopy accessories



Milestone's Clean Chemistry accessories are designed to reduce and control the analytical blank in ultratrace elemental analysis. According to the company, duoPUR and subCLEAN provide on-demand, in-house purification of acids, and traceCLEAN is an automated self-contained acid steam cleaning system for trace metal analysis accessories.

Milestone Inc.,
Shelton, CT;
www.milestonesci.com/CleanChemistry

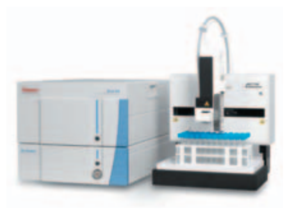
IR transmission analysis accessory



The *Pearl,* a liquid infrared transmission analysis accessory from Specac, is designed with a horizontal liquid cell (the Oyster Cell) and a replaceable lower window that allows users to customize the pathlength. According to the company, the liquid cell can be set at a wedged angle to avoid any fringing pattern in background readings.

Specac Ltd,
London, UK, and Philadelphia, PA;
www.specac.com

Infrared spectrometer



Thermo Fisher's Delta Ray isotope ratio infrared spectrometer (IRIS) is designed to facilitate interfacing with samples available in amounts as little as 80 µg of CO_2, as in vials, syringes, or bags. According to the company, the spectrometer extends the continuous measurement of isotope ratios and concentrations of CO_2 in air to discrete samples in applications such as dissolved inorganic carbon measurement, carbonate isotope ratio determination, and microbiology labeling experiments.

Thermo Fisher Scientific, San Jose, CA;
www.thermoscientific.com

Raman Spectroscopy and Imaging of Low-Energy Phonons in Solid State Materials

LIVE WEBCAST: Thursday, June 16, 2016 at 10 am PDT | 12 pm CDT | 1 pm EDT

Register for free at www.spectroscopyonline.com/spec/imaging

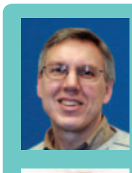
EVENT OVERVIEW

Raman bands in the low-energy region of the spectrum of crystals are attributed to so-called external lattice vibrational modes. The Raman bands from these external vibrational modes (low-energy phonons) are very sensitive to crystal structure and orientation with respect to the incident laser polarization and to molecular interactions within the crystal. We will present results demonstrating the use of low-energy Raman spectroscopy to probe solid state materials and chemical bond interactions.

Key Learning Objectives:

- The sensitivity of low-energy phonons to the structure of 2D crystals
- The complementarity of reflected light and low-energy Raman imaging
- The probing of chemical bond interactions through the Raman band structure of low-energy phonons

Presenters



David Tuschel
Manager of Raman Applications
HORIBA Scientific

Moderator:
Laura Bush
Editorial Director
Spectroscopy

Who Should Attend:

- Pharmaceutical scientists
- Materials scientists
- 2D crystal device engineers and scientists

Sponsored by HORIBA Scientific

Presented by Spectroscopy

For questions, contact Kristen Moore at kmoore@advanstar.com

Calendar of Events

May 2016

25–28 3rd International Conference on New Trends in Chemometrics and Applications (NTCA 2016)
Side-Antalya, Turkey
ntca.ankara.edu.tr/

29–3 June 40th International Symposium on Capillary Chromatography and 13th GCxGC Symposium
Riva del Garda, Italy
192.167.108.132/slider.html

June 2016

3–4 Symposium on Application of Fundamental Parameters in X-ray Analysis
Ontario, Canada
www.uwo.ca/earth/xrfcourse/symposium.html

5–9 64th ASMS Conference on Mass Spectrometry & Allied Topics
San Antonio, TX
www.asms.org/conferences/annual-conference/annual-conference-homepage

5–10 CLEO 2016: Laser Science to Photonic Applications
San Jose, CA
www.cleoconference.org/home/

15–17 6th Baltic Electrochemistry Conference
Helsinki, Finland
chemistry.aalto.fi/en/current/6th_electrochemistry_meeting/

19–24 European Conference on X-Ray Spectrometry (EXRS) 2016
Gothenburg, Sweden
exrs2016.se/

26–30 SPEC 2016
Montréal, Canada
www.spec2016.com/

27–29 2nd International Conference on Integrated Functional Nano Systems
Graz, Austria
www.nanofis.net/

27 June–1 July 15th Meeting of the European Society of Sonochemistry (ESS-15)
Istanbul, Turkey
ess2016istanbul.org/

July 2016

2–9 NANOTEXNOLOGY 2016
Thessaloniki, Greece
www.nanotexnology.com/

3–7 12th EUROMAR 2016 Conference: A European Magnetic Resonance Meeting
Aarhus, Denmark
www.euromar.org/

25–27 ANM2016: 7th International Conference on Advanced Nanomaterials, 2nd International Conference on Graphene Technology, and 1st International Conference on Spintronics Materials
Aveiro, Portugal
www.anm2016.com/

25–28 Applied Industrial Optics (AIO)
Heidelberg, Germany
www.osa.org/en-us/meetings/optics_and_photonics_congresses/imaging_and_applied_optics/applied_industrial_optics/

25–29 16th International Conference on Organized Molecular Films (ICOMF16)
Helsinki, Finland
www.helsinki.fi/icomf16/index.html

August 2016

1–5 Denver X-ray Conference 2016
Rosemont, IL
www.dxcicdd.com/16/index.htm

8–12 National Environmental Monitoring Conference (NEMC)
Orange County, CA
nemc.us/index.php

21–24 NZIC-16: New Zealand Institute of Chemistry Conference
Queenstown, New Zealand
www.nzic16.org/

31 August–2 September Ultrafast Imaging of Photochemical Dynamics: Faraday Discussion
Edinburgh, UK
www.rsc.org/events/detail/19765/

October 2016

5–6 Cannabis Science Conference (CANNCON 2016)
Portland, OR
www.cannabisscienceconference.com/

17–21 Frontiers in Optics/Laser Science (APS/DLS)
Rochester, NY
www.frontiersinoptics.com/home/

30–4 November Advanced Solid State Lasers Conference and Exhibition
Boston, MA
assl.osa.org/home/

November 2016

14–16 2016 Eastern Analytical Symposium and Exposition
Somerset, NJ
eas.org

Short Courses

June 2016

4–5 MS/MS: An Introduction to Instrumentation, Fundamentals, and Spectral Interpretation
San Antonio, TX
www.asms.org/docs/default-source/conference-short-course-descriptions/10-ms-ms-intro-revised.pdf?sfvrsn=2

5 SC149 - Foundations of Nonlinear Optics
San Jose, CA
www.cleoconference.org/home/program/short-courses/sc149/

5 SC301 - Quantum Cascade Lasers: Science, Technology, Applications, and Markets
San Jose, CA
www.cleoconference.org/home/program/short-courses/sc301/

5 SC361 - Coherent Mid-Infrared Sources and Applications
San Jose, CA
www.cleoconference.org/home/program/short-courses/sc361/

6 SC424 - Optical Terahertz Science and Technology
San Jose, CA
www.cleoconference.org/home/program/short-courses/sc424/

6–17 XRF Short Course
Ontario, Canada
www.uwo.ca/earth/xrfcourse/xrf_2016/registration.html

13–17 Interpretation of Infrared and Raman Spectra
Coventry, UK
www.ircourses.org/

15–17 X-ray Photoelectron Spectroscopy (XPS/ESCA) and Data Processing
Dayton, OH
www.surfaceanalysis.org/

21–23 A107 | Fourier Transform Infrared Spectroscopy (FTIR) Operations and Maintenance
Franklin, MA
https://www.signup4.net/Upload/THER15A/2016562E/EPM_Training-ParticulateSamplers_F.pdf

July 2016

11–15 Interpretation of Infrared and Raman Spectra
Brunswick, ME
www.ircourses.org/

Spectroscopy EDITORS' SERIES

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Forensic Applications of Isotope Ratio Mass Spectrometry

ON-DEMAND WEBCAST Originally aired April 19, 2016

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EVENT OVERVIEW:

The isotopic profile of a material refers to the ratios of the stable isotopes of elements contained within, such as ^{2}H/^{1}H, ^{13}C/^{12}C, and ^{18}O/^{16}O. Biological, chemical and physical processes cause variations in the ratios of stable isotopes; analysis of a material for its distinctive isotopic signature can thus be used to reveal information about its history. Isotope ratio mass spectrometry (IRMS) is a technique used to measure the relative abundance of isotopes in materials. Forensic investigators have used IRMS to measure a variety of materials, such as drugs, explosives, food, and human remains. This web seminar will discuss the use of IRMS in forensic science and include several case examples.

Key Learning Objectives:

- How isotope ratio mass spectrometry (IRMS) can be used to measure the relative abundance of isotopes in materials
- Best practices for effective use of the technique
- Examples from the use of IRMS in forensic science

For questions, contact Kristen Moore at kmoore@advanstar.com

Presenter

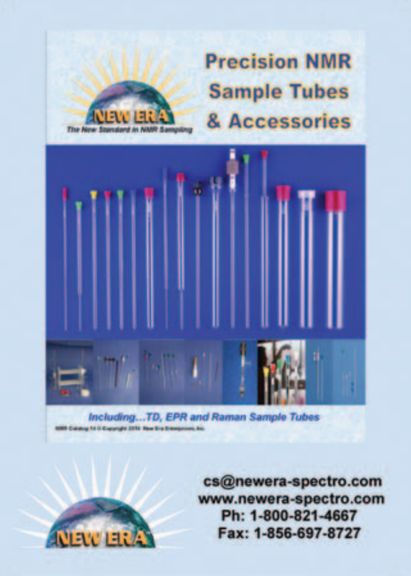
Lesley A. Chesson
President
IsoForensics, Inc.

Moderator:
Laura Bush
Editorial Director
Spectroscopy

Who Should Attend:

- Forensic scientists and members of the broader law enforcement and judicial community looking to better understand the use of isotope-ratio mass spectrometry in forensic use
- Anyone interested in learning more about the use of IRMS for other fields, such as determining the origin of food and beverages

Spectroscopy SHOWCASE



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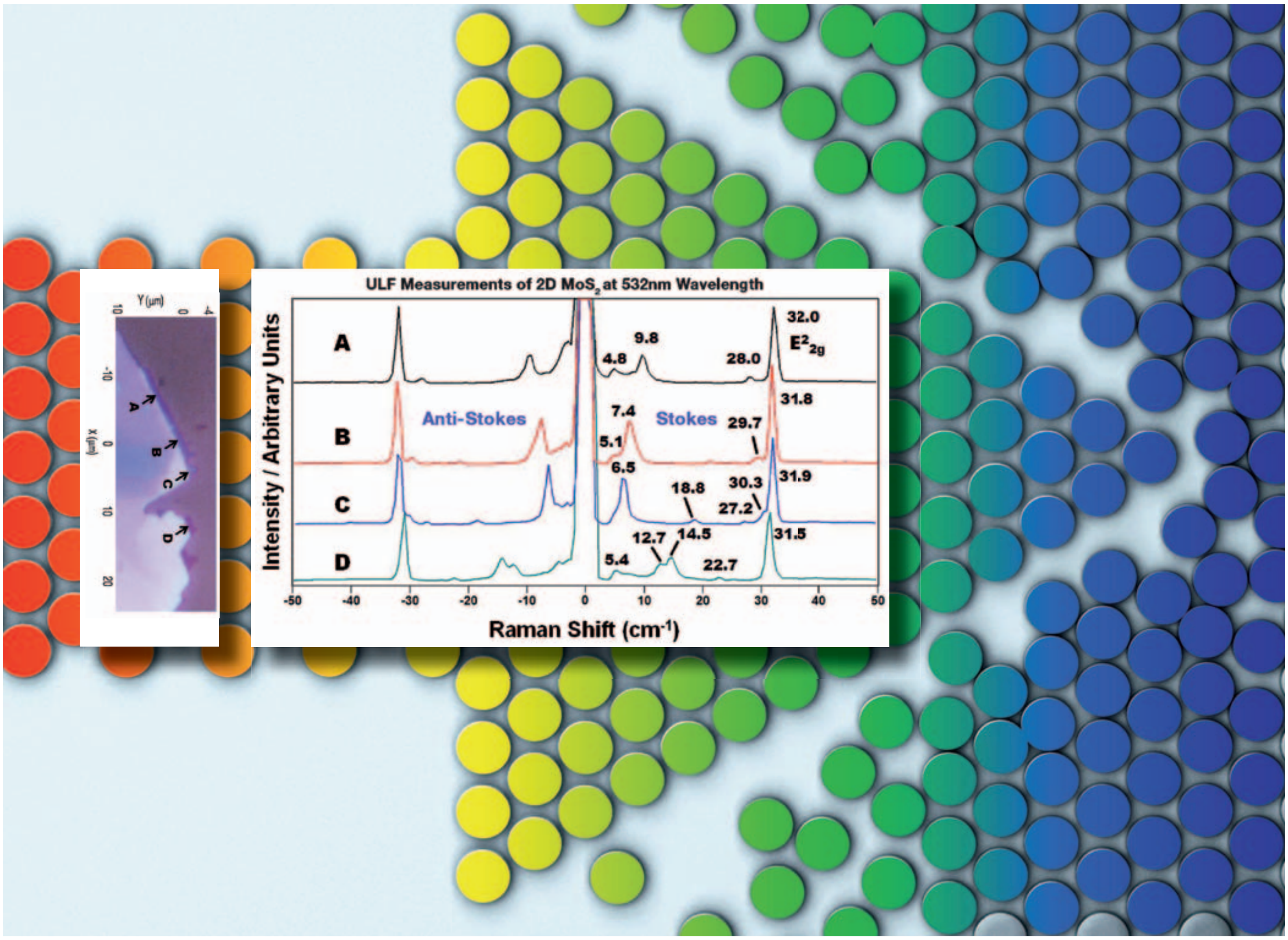
Raman Spectroscopy and Imaging of Low-Energy Phonons in Solid State Materials
Thursday, June 16 at 1 PM EDT / 10 AM PDT
http://www.spectroscopyonline.com/spec/imaging



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