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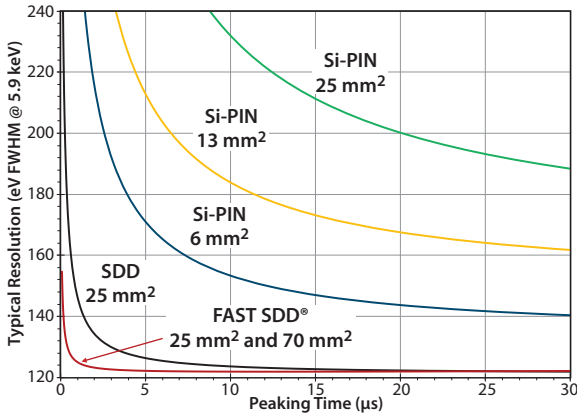
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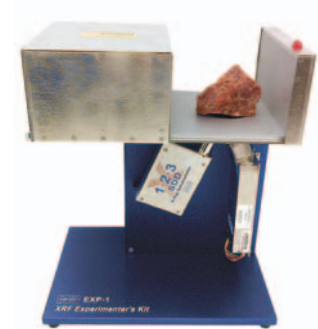
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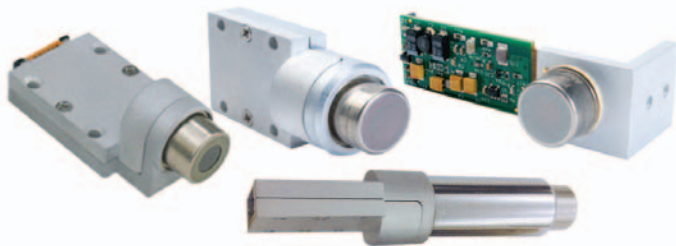


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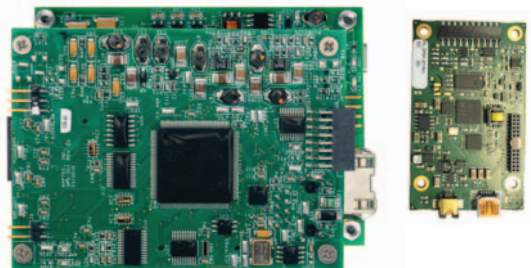


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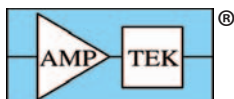
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ON THE WEB

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 22 of this issue or at:

www.spectroscopyonline.com/ir-spectral-interpretation-workshop-0

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CONTENTS

COLUMNS

Atomic Perspectives 14

From Heavy Metals Testing to the Measurement of Elemental Impurities in Pharmaceuticals: Over 100 Years in Making the Change

Tony DeStefano and Robert Thomas

A look at the implementation of the new *United States Pharmacopeia (USP)* chapters and the *International Conference for Harmonization (ICH)* guidelines for elemental impurities from an historical perspective, providing insight into the changes and considering the challenges and opportunities that lie ahead as the industry embraces the new methodology.

IR Spectral Interpretation Workshop 20

The Carbonyl Group, Part V: Carboxylates—Coming Clean

Brian C. Smith

Carboxylates are made by reacting carboxylic acids with strong bases such as inorganic hydroxides. Carboxylates contain two unique carbon–oxygen “bond and half” linkages that coordinate with a metal ion to give two strong infrared peaks, which make them easy to see.

Spectroscopy Spotlight. 24

Understanding Molecular Interactions with Advanced FT-IR Spectroscopy and Imaging

An interview with Sergei G. Kazarian

Fourier transform infrared (FT-IR) and attenuated total reflection (ATR)-FT-IR spectroscopic imaging are important tools for understanding molecular interactions. Sergei G. Kazarian of Imperial College London has used these advanced imaging techniques in a wide range of applications.

FEATURE

Review of New Spectroscopic Instrumentation for 2018 28

Howard Mark and Mike Bradley

Our annual review of spectroscopy products, broken down into the following categories:

Atomic Spectroscopy	33
Fluorescence	34
Mass Spectrometry	35
Mid-IR	36
NIR	37
NMR and ESR	39
Raman	39
UV-vis	41
X-ray	41
Software	41
Accessories	45
Components	48

DEPARTMENTS

News Spectrum	10–12	Short Courses	56
Products & Resources	52	Call for Papers	57
Calendar	55	Ad Index	58

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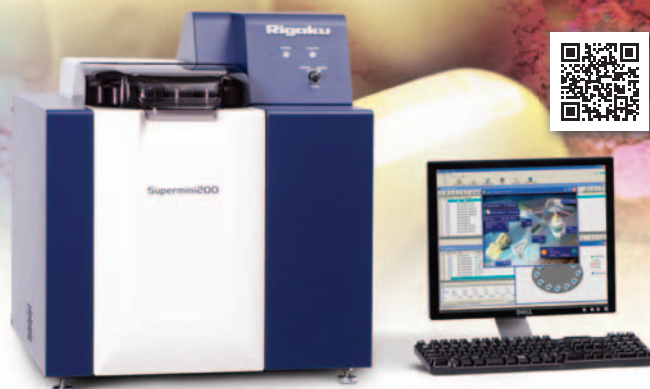
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News Spectrum

Specac Wins Queen's Award for International Trade

Specac Limited, a provider of accessories for infrared and X-ray spectroscopy, has won the Queen's Award for Enterprise, in the category of International Trade. England's Queen Elizabeth II has approved the prime minister's recommendation for the award.

David Smith, managing director of Specac, said that he was deeply honored that the business has won such a prestigious award. "I believe it represents recognition at the highest level for a good commercial strategy, high quality in everything we design and make, and mostly, the hard work over a long period of an amazing team," he said.

Jo Johnson, a member of parliament for Orpington, Kent, where Specac is located, and the minister of state at the Department of Transport, and until recently, minister of state for Universities and Sciences said, "It is fantastic news that Specac has been recognized for its considerable contribution to international trade at the Queen's Awards for Enterprise." He added that the award is an outstanding achievement of which the company and its employees should be very proud.

In a statement, Specac expressed appreciation of its key partners, both suppliers and customers. "We are a hugely ambitious business, and we consider the success we've achieved as merely a beginning," the statement continued. "We welcome new, collaborative partners as we expand our horizons and try to help more scientists to resolve their applications needs."

Specac works with original equipment manufacturers and a worldwide distribution network, as well as industrial, academic, and government customers. The company designs and manufactures its products at its facility in Orpington, Kent, on the outskirts of London. Sales offices are located in the United States, China, and Singapore.

In addition to international trade, the Queen's Award for Enterprise also recognizes outstanding achievement by United Kingdom businesses in three other categories: innovation, sustainable development, and promoting opportunity through social mobility.

Bruker Acquires Anasys Instruments

Bruker Corporation (Billerica, Massachusetts) has acquired Anasys Instruments Corporation, a privately held company that develops and manufactures nanoscale infrared (nano IR) spectroscopy and thermal measurement instruments such as atomic force microscopy and white-light interferometric three-dimensional (3D) microscopy. The acquisition extends Bruker's portfolio of Raman and Fourier-transform IR (FT-IR) spectrometers and its nanoscale science instruments.

Anasys, headquartered in Santa Barbara, California, provides products used for nanoprobe-based thermal

and infrared measurements. The company's nanoIR products are used by academic and industrial scientists, by engineers in soft-matter and hard-matter materials science, and in life science applications. Recently, Anasys introduced 10-nm resolution nanoIR imaging.

Mark R. Munch, president of the Bruker Nano Group, said the company is excited to add this high-growth area to its portfolio of nanoscale microscopy and spectroscopy measurement products. "There are tremendous application and technology synergies that will benefit our customers," he said.

"We are very happy to have found a company like Bruker to take the business to the next level," said Roshan Shetty, cofounder and former CEO of Anasys.

IR QUIZ TIME

Your latest interpretation problem is seen in the figure below. Using everything you have learned from the March installment of "IR Spectral Interpretation Workshop" and previous columns, determine the functional groups present and try to discover the chemical structure of this compound. Remember that not all peaks will be useful in the structural determination.

To see the answer, please turn to page 22.

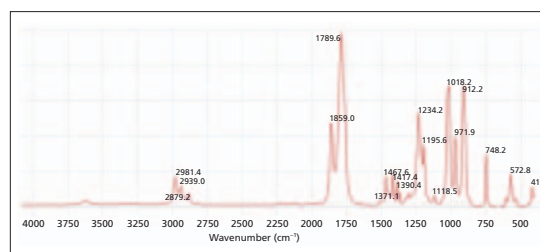


Figure: The IR spectrum of a solid. Thin film melt.

Table: Peak positions for the problem spectrum

2981	1859	1417	1234	748
2939	1789	1390	1018	572
2879	1467	1371	918	

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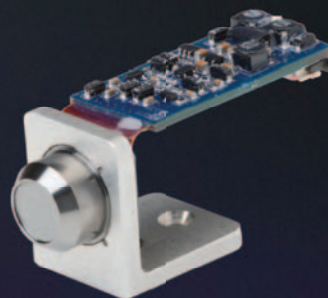
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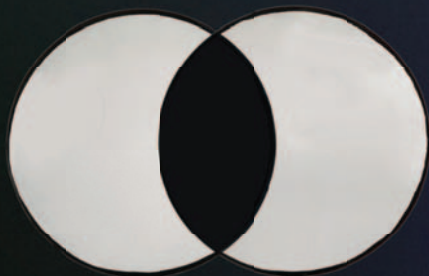
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Unique Challenges of Forensic Science Highlighted at Local SAS Meeting

By Debbie Peru

The March meeting of the New York–New Jersey Chapter of the Society for Applied Spectroscopy (NYSAS) was held on March 28 in the Ceramics Research building at Rutgers University. The invited speaker was Professor John A. Reffner of John Jay College of Criminal Justice in New York, New York. The meeting was hosted by Professor Laura Fabris of the Department of Materials Science and Engineering at Rutgers.

Reffner's scientific interests are focused on uniting microscopy with spectroscopy and applying novel technologies for advancing both materials and forensic science. He pioneered the development of infrared (IR) microspectrometers and innovative applications of IR microprobe technology for forensic applications. Among Reffner's scientific accomplishments, he has received many prestigious scientific awards including the American Society of Trace Evidence Examiners' Edmond Locard Award (2016), The Society of Applied Spectroscopy's Gold Medal Award (2015), and the American Academy of Forensic Sciences' Paul L. Kirk Award (2004). Reffner has also served as a consultant to the Connecticut State Police for more than 25 years, and has testified as an expert witness in criminal, civil, and patent litigations.

Reffner's presentation focused on how combinations of analytical techniques are being used in forensic investigations. Today, Reffner noted, forensic science is under attack by defense attorneys, judges, and public advocates. Police departments, government agencies, and social groups are challenging the validity of the testimonies of expert witnesses. Some academics and scientists also question the way in which forensic laboratories analyze evidence and interpret the results of their studies. As a result, demands on forensic scientists are increasing daily.

In this context, there has been a call to standardize analytical methods used in the crime laboratories and spectroscopy has become an essential technology for elevating the quality of forensic evidence analysis. Reffner's presentation included highlights of many interesting forensic cases that he has been involved in, including authenticating a winning lottery ticket, matching red fibers in a murder investigation, identifying the chemical makeup of a multilayer paint chip being used as evidence in a hit and run case, and identification of adhesive residue found on a suspect's knife.

The meeting was attended by many students and several university professors, as well as by consultants and industrial members. The students were encouraged to ask questions and received an engraved pen for participation in the question-and-answer session following the talk.

During the dinner section of the meeting, several students from Fabris's group displayed posters. The posters highlighted optimization and applications of surface-enhanced Raman spectroscopy (SERS) and facilitated interesting discussions between the students and industrial attendees.

More information about the chapter and the schedule of meetings can be found at www.nysas.org.

Approach Combining FT-IR and LA-ICP-MS Provides Improved Tissue Classification

A recent study used a combined chemical analysis approach to investigate rat brains harvested one week after induction of photothrombotic stroke (1). Researchers from Austria, the Netherlands, and Qatar used Fourier transform infrared (FT-IR) spectroscopy and laser ablation inductively coupled plasma–mass spectrometry (LA-ICP-MS) for the imaging of cerebral ischemia to obtain a deepened analysis compared to single techniques or side-by-side analysis.

The LA-ICP-MS data were normalized using an internal standard (a thin gold layer). Hyperspectral data cubes that were acquired were fused and subjected to multivariate analysis. Brain regions affected by stroke as well as unaffected gray and white matter were identified and classified using a model based on either partial least squares discriminant analysis (PLS-DA) or random decision forest (RDF) algorithms.

According to the researchers, the RDF classifier built on the combined data sets appeared to be more precise compared to classifiers built on the individual data sets. They concluded that multisensory hyperspectral imaging with subsequent RDF-based analysis can deepen the understanding of biochemical processes in ischemic brains and enable automated identification of different types of tissues.

Reference

- (1) A. Balbekova, H. Lohninger, G.A.F. van Tilborg, R.M. Dijkhuizen, M Bonta, A Limbeck, B. Lendl, K.A. Al-Saad, M. Ali, M. Celikic, and J. Ofner, *Appl. Spectrosc.* **72**(2), 241–250 (2018). ■

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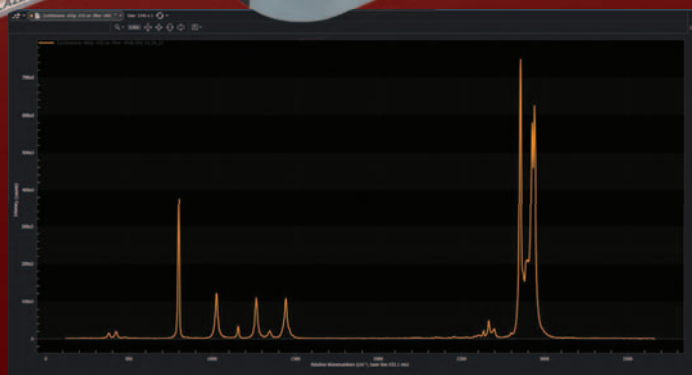
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Atomic Perspectives

From Heavy Metals Testing to the Measurement of Elemental Impurities in Pharmaceuticals: Over 100 Years in Making the Change

As a follow up to March 2018's "Atomic Perspectives" column, which provided guidance on how to choose the optimum technique for carrying out the measurement of elemental impurities in pharmaceuticals, this month's installment takes a look at the implementation of the new *United States Pharmacopeia (USP)* Chapters and the *International Conference for Harmonization (ICH)* guidelines for this method from an historical perspective. This column provides insight into these changes and takes a look at the challenges and opportunities that lay ahead as the industry embraces this new methodology.

Tony DeStefano and Robert Thomas

The identification and quantification of elemental impurities in pharmaceuticals have been a challenge for many years. In the late 1800s and early 20th century, lead was an issue because it was used in the production of solder, and, absent the good manufacturing practices controls that are in place today, metals from manufacturing and processing equipment posed potential problems, as did mined excipients that could carry with them elements such as arsenic, lead, cadmium, and mercury.

The United States Pharmacopeia (USP) first addressed this issue in 1908, with the publication of what became general chapter <231> - Heavy Metals. This test typically involves the high-temperature digestion of the material of interest followed by sulfide precipitation of the metals of interest. The specification is based on comparison of the color of the resulting precipitate to the color of a lead sulfide precipitate prepared at the level of interest (typically 10 or 20 ppm). There are, of course, many issues with this test. The test generates hydrogen sulfide, which can be highly toxic, and

in the USP method, does this through the use of thioacetamide, which has its own safety issues. The test was initially designed to detect lead, mercury, bismuth, arsenic, antimony, tin, cadmium, silver, copper, and molybdenum. Not included are common components of manufacturing equipment such as nickel and vanadium, or common catalysts such as platinum or palladium. In addition, the test is a screening test and is not element specific, and since each precipitate has a different color (and most are lighter than the color of lead sulfide), even its use as a total metal limits test can be questioned. A final issue is that the test is based on visual acuity, rather than being toxicologically based. For a test for elements considered toxic, it is far preferred that it be based not on what one observes, but rather on what levels are of toxicological concern.

The Process for Change

Given all these issues, why did the test remain as an official test in the USP until January 2018, approximately 110 years after its introduction? The primary reason is likely that there was not an



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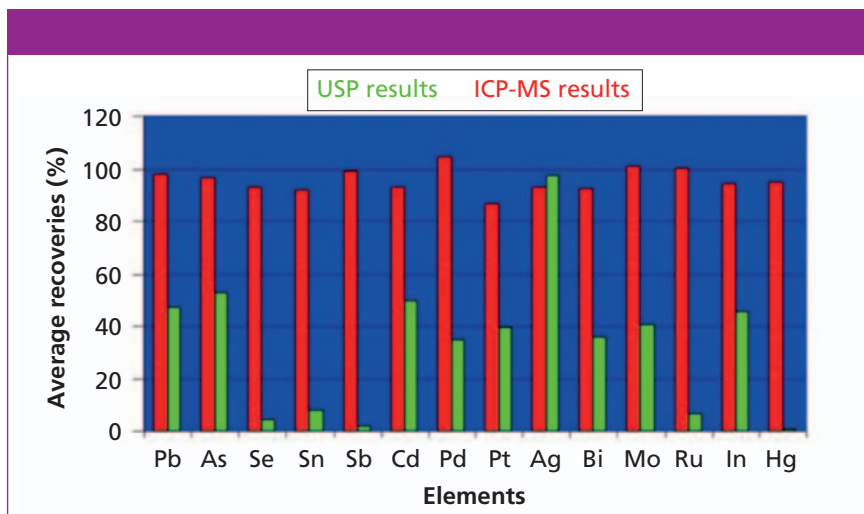


Figure 1: Comparisons between ICP-MS and Method II described in *USP* Chapter <231> (3).

industry-wide, globally accepted test to replace it. For all its faults, the methodology of general chapter <231> was well understood, routinely used by the industry, and was harmonized with the European and Japanese pharmacopeias. The winds of change began with the publication in 1995 of a Stimuli to the Revision Process article in the *Pharmacopeial Forum* by Katherine Blake (1). In this article, she noted that often 50% of the metal of interest was lost in the ash process, and that there was essentially zero recovery for mercury, one of the more toxic and common elements of interest. In 2000, Dr. Taibang Wang made similar observations in an article in the *Journal of Pharmaceutical and Biomedical Analysis*, where he noted “Although still widely accepted and used in the pharmaceutical industry, these methods based on the intensity of color of sulfide precipitation are non-specific, labor intensive, and more often than hoped, yield low recoveries or no recoveries at all” (2). Then, in 2004, Nancy Lewen and coworkers directly compared the recoveries of 14 elements using *USP* <231> Method II and inductively coupled plasma-mass spectrometry (ICP-MS). Consistent with the other two articles, this study showed a number of recoveries around 50%, with recoveries of less than 10% for Se, Sn, Sb, and Ru with, as anticipated, no recovery at all for Hg, as exemplified in Figure 1 (3).

USP Expert Committees

This work set the stage for the establish-

ment at *USP* of a series of committees and expert panels, beginning in earnest with the 2005–2010 revision cycle to update the concept of heavy metals testing. The process built on an Institute of Medicine meeting commissioned by *USP* in 2008, and on a document issued by the European Medicines Agency (EMA), which developed guidelines on the control of residual catalysts in pharmaceuticals with the goal of establishing limits based on toxicological safety assessments of common catalytic elements. This work began as early as 1998 and resulted in a guideline that was officially implemented in 2008 (4).

ICH Involvement

Building on all this, *USP* published in the *Pharmacopeial Forum* a proposed general chapter on Inorganic Impurities: Heavy Metals that was the early precursor to general chapter <232> - Elemental Impurities – Limits, and <233> - Elemental Impurities – Procedures (5). This *USP* initiative led to the desire by the pharmaceutical industry participants to have, as with general chapter <231>, a chapter that was harmonized across the pharmacopeias in the International Conference for Harmonization (ICH) region (at a minimum, the United States, Europe, and Japan). The result of this harmonization initiative was the ICH Q3D expert working group, and the final output was the *ICH Q3D* guideline on elemental impurities, with the step 4 document posted to the ICH website in December 2014 (6).

The guideline was implemented for new drug products by the U.S. Food and Drug Administration (FDA) beginning in July, 2016, and for all drug products, new and existing, in the *USP* in January 2018, concurrent with omission from the *USP* of general chapter <231>. General chapter <232> applies only to drug products and not to drug substances or excipients, since without knowledge of issues such as dose and route of administration, establishment of specifications for these materials is not possible.

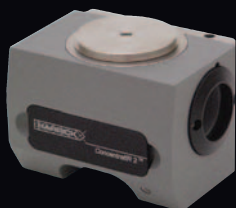
ICH Q3D focused on the establishment of a list of elements of toxicological concern and their limits in oral, parenteral, and inhalational dosage forms as well as a risk-based approach for demonstrating absence of the various metals and compliance with the specification. An extensive body of training materials is available to help practitioners understand the scope of the guideline, the concept of a risk-based approach, and how to think about issues such as the calculations of concentrations in the drug product and extension to other dosage forms (7). Because the entire process is risk based, testing is only one of many ways by which compliance with the standard can be demonstrated. The full list of permitted daily exposure (PDE) elemental limits defined in *USP* Chapter <232> and the *ICH Q3D* Step 4 guideline are shown in Table I. Note that the classification is based on their toxicological impact (a combination of toxicity and likelihood of occurrence), with Class 1 and 2A elements considered the most significant.

Testing of drug products and excipients was not discussed in detail by the ICH Q3D working group. Rather, it was left to the individual pharmacopeias to work out their own procedures, with the goal of long-term harmonization of the final results. In the *USP*, general chapter <233> describes two procedures, inductively coupled plasma-optical emission spectroscopy (ICP-OES) and ICP-MS, along with system suitability and validation requirements for these tests and any alternative tests. It is noted that any test that meets the validation requirements and is otherwise fit for purpose can be used instead of the two proposed tests.

The implementation of the *ICH Q3D* guideline and the two *USP* general chap-

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Table 1: Permitted daily exposure (PDE) limits as defined in USP Chapter <232> and the ICH Q3D Step 4 guideline

Element	Class	Oral PDE (µg/day)	Parenteral PDE (µg/day)	Inhalational PDE (µg/day)
Cd	1	5	2	2
Pb	1	5	5	5
As	1	15	15	2
Hg	1	30	3	1
Co	2A	50	5	3
V	2A	100	10	1
Ni	2A	200	20	5
Tl	2B	8	8	8
Au	2B	100	100	1
Pd	2B	100	10	1
Ir	2B	100	10	1
Os	2B	100	10	1
Rh	2B	100	10	1
Ru	2B	100	10	1
Se	2B	150	80	130
Ag	2B	150	10	7
Pt	2B	100	10	1
Li	3	550	250	25
Sb	3	1200	90	20
Ba	3	1400	700	300
Mo	3	3000	1500	10
Cu	3	3000	300	30
Sn	3	6000	600	60
Cr	3	11,000	1100	3

ters, and the elimination of USP <231> are major steps forward in the analysis of elemental impurities in pharmaceuticals. There is now broad agreement across the pharmaceutical industry and across many countries about the elements of toxicological concern and the levels at which they should be controlled.

Why Did This Process Take So Long?

Let's get back to the earlier question: Why did it take 110 years to get here? The simple answer is that it took that amount of time and innovation for the right technology to be developed and for the technology to be widely available and accepted by the pharmaceutical in-

dustry. For a drug product specification to be accepted as a public standard (as opposed to a private standard between a pharmaceutical company and a regulatory body where the company can perhaps propose a sophisticated test not readily available), any proposed test needs to be well established, well accepted by the industry, reliable, and broadly available, either in house or through contract research organizations.

Until the last several years, these requirements simply hadn't been met. Only a few technologies are capable of meeting the requirements of general chapters <232> and <233>. While ICP-OES was widely available, there are situations, especially for low-dose drugs or par-

enteral or inhalational drugs, where a number of elements need to be measured or controlled; ICP-MS is the option of choice. Only recently have the software, hardware, price, and availability—either in house or through contract research organizations—been there to make broad applicability across the industry feasible.

In addition, a suite of new technologies, sampling accessories, and data processing tools is making life easier for pharmaceutical companies that are working in a good manufacturing practice (GMP) environment. Some of these are aimed at laboratories that are looking to maximize sample throughput by using productivity enhancement tools to automate the full suite of quality control and spike recovery testing procedures described in Chapter <233>, as well as to ensure that the calculations are done correctly and properly documented, in order to minimize operator interaction, and allow the analyst to focus on other tasks.

Other areas that have been addressed include software tools to provide data in a suitable compliant form for regulatory submission and inspection. For example, any analytical instrument used for measuring pharmaceuticals must also comply with the FDA's 21 CFR Part 11 regulations to ensure the integrity of any electronic records that are generated. The instrument's software control and data handling must therefore incorporate tools to maintain the integrity of the analytical method and subsequent results and provide transparency to data generation, including support for audit trails as well as security features to ensure that alterations cannot be made without a clear explanation of the process. It's therefore very important that the instrument and its software provide the necessary support to meet these kinds of demands in the highly regulated pharmaceutical industry environment.

Risk Assessment

The widespread availability of this technology, and the study and publication of results of the levels of elemental impurities in drug substances and excipients will likely lead to less testing of materials in the long run. Currently, many drug substances and excipients are being tested for the first time. As databases

are developed and made public, many excipients and drug substances may be demonstrated to be of sufficiently low concern that they will no longer need to be considered in a risk assessment, and risk assessments may be limited to perhaps a few specific mined excipients, or materials used in very high quantities in a dose form. Thus testing, which is already only one part of an overall risk assessment, may become even less frequent in the future. This development is an example of the technology providing a breakthrough in the assessment of safety, and soon being relegated to a role as a tool for specific purposes and very seldom, if ever, as a tool for routine monitoring of drug products.

What's left to get to the point where the industry feels that the risks of elemental impurities are well understood and controlled and only minimal levels of testing are necessary? A key piece will be accurate measurement of the levels of elemental impurities in drug substances and excipients, and the broad availability of this information. Another key to making this happen is the generation of good data by the people producing data on the various drug substances, excipients, and drug products. The industry needs good data upon which to make decisions, and the generation of such data for elemental impurities is quite difficult. Issues such as sample homogeneity, sample contamination, instrument sensitivity, and instrument artifacts all play a role in the generation of reliable data.

Sample contamination is of particular concern. As discussed above, the elements of most concern (for example, As, Pb, Cd, Hg, Ni, V, and Co) have been selected because they are both potentially toxic and widely found in the laboratory or in nature, whether in glassware, equipment, reagents, or even clothing or accessories worn by analysts or others in the laboratory. Accessories containing metals can be of particular concern. In addition, reagents such as concentrated acids need to be tested to be free of metals to avoid sample contamination. At the trace levels at which these elements are being detected, very low levels of contamination can lead to false positive results, which in turn can result in additional testing and rework.

Similarly, ICP-MS instrumental artifacts can also lead to erroneous results, such as the effect of the $^{40}\text{Ar}^{35}\text{Cl}$ polyatomic spectral interference on the measurement of ^{75}As . This effect is of particular concern if chloride is present in the sample matrix or if concentrated hydrochloric acid is used for the digestion of the sample. The chloride ions will combine with the argon from the plasma to form an argon chloride spectral interference that will significantly interfere with the monoisotopic arsenic ion at mass 75. This effect can be minimized by avoiding hydrochloric acid in the digestion procedure, but if this is not possible, or chloride is present in the drug product, an ICP-MS system fitted with a collision–reaction cell is a very important tool to have at your disposal to help prevent the formation of the interference.

In Summary

We have come a long way in the assessment of risk of toxicity from low-level trace elements in pharmaceuticals from the days of sulfide precipitation and comparison to a lead sulfide standard. The new risk assessment strategies and tools—such as closed-vessel digestion to provide analyzable samples with minimal analyte loss and ICP-MS to provide the requisite sensitivity and selectivity—have enabled the industry to quantify the elemental impurity levels in drug substances, excipients, and drug products and reach a point where solid, risk-based assessments can be made with only minimal testing needed in the long term.

This month's column has been adapted from Robert Thomas's new book (8).

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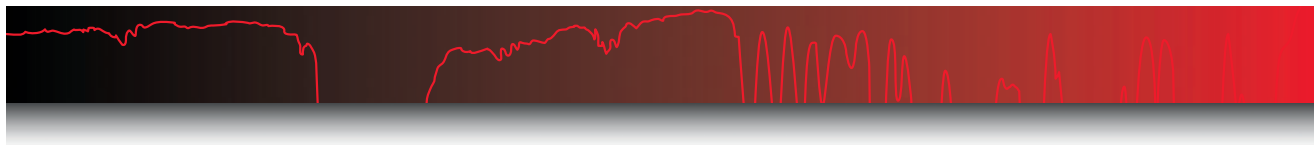
former Vice President at US Pharmacoepia, he led the initiatives to maintain, update, and redesign the General Chapters, and also served as a member of the ICH Q3D Expert Working Group on metal impurities. He has advanced degrees in Physical Chemistry from Cornell University and is a member of the American Chemical Society (ACS) and past president of the American Association of Pharmaceutical Scientists (AAPS).



Robert Thomas is principal of Scientific Solutions, a consulting company that serves the application and writing needs of the trace element user community. He has

worked in the field of atomic and mass spectroscopy for more than 40 years and has written over 80 technical publications including a 15-part tutorial series on ICP-MS. He recently completed his fourth textbook entitled *Measuring Elemental Impurities in Pharmaceuticals: A Practical Guide*. He has an advanced degree in analytical chemistry from the University of Wales, UK, and is also a Fellow of the Royal Society of Chemistry (FRSC) and a Chartered Chemist (CChem). He has served on the ACS Committee on Analytical Reagents for the past 17 years.

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IR Spectral Interpretation Workshop

The Carbonyl Group, Part V: Carboxylates—Coming Clean

Carboxylates are made by reacting carboxylic acids with strong bases such as inorganic hydroxides. The resultant salts are commonly used as cleansers, including in common bar soap—hence the pun in the title. Carboxylates contain two unique carbon–oxygen “bond and half” linkages that coordinate with a metal ion to give two strong infrared peaks, which make them easy to see.

Brian C. Smith

So far in our investigation of the infrared spectroscopy of the carbonyl functional group, we have looked at ketones, aldehydes, carboxylic acids, and acid anhydrides (1–4). Acid anhydrides are derivatives of carboxylic acids and are made by reacting two acid molecules and splitting off an atom of water (4). Carboxylates are another derivative of carboxylic acids, and they are made via a classic acid–base reaction of a carboxylic acid with a strong base such as a hydroxide. Such a reaction is shown in Figure 1.

As in the synthesis of acid anhydrides, one of the driving forces for the reaction is the splitting-off of a molecule of water. Note in Figure 1 that the carboxylate functional group contains ionic bonding; there is a formal positive charge on the metal ion and a negative charge on the carboxylate. Also shown in Figure 1 is that the metal ion from the hydroxide coordinates with the two oxygens from the carboxylic acid to form an unusual bonding arrangement with two equivalent carbon–oxygen bonds. We will call this the “ $-\text{CO}_2^-$ ” group because it contains two carbon–oxygen bonds of the same bond order, similar to carbon dioxide ($\text{O}=\text{C}=\text{O}$).

Carboxylates are named after the acid and base used to make them. Thus, the reaction of acetic acid and sodium hydroxide would yield sodium acetate. A classic acid–base reaction, such as between NaOH and HCl,

forms a salt and water. Carboxylates are sometimes referred to as *carboxylic acid salts* because a carboxylate is a salt formed by the reaction of a carboxylic acid with a base.

Carboxylates are unusual in that they frequently have a polar end consisting of the carboxylate, and a nonpolar end such as an alkyl chain. This structure makes them uniquely capable of solubilizing oil and dirt into water, which is why they are commonly used as cleaning agents (explaining the bad pun in the title of this column). In fact, sodium stearate, the product of the reaction of sodium hydroxide and stearic acid, is also known as hand soap.

The infrared spectrum of a carboxylate, zinc stearate, is shown in Figure 2. This molecule is made by reacting two equivalents of stearic acid with the dibasic zinc hydroxide, yielding a molecule with two carboxylate moieties.

Because carboxylates contain neither a $\text{C}=\text{O}$ bond nor a $\text{C}-\text{O}$ bond, they will not contain a carbonyl stretching peak around 1700 cm^{-1} (1) (going forward assume all peak positions are in wavenumber units), or a $\text{C}-\text{O}$ stretch between 1300 and 1000 (5). There are two intense peaks at 1538 and 1398 in Figure 2 that stick down out of the spectrum like canine teeth. These are from the asymmetric and symmetric stretches of the $-\text{CO}_2^-$ group. Generally, these

two peaks fall from 1650 to 1540 and 1450 to 1360, respectively. Unlike the C=O group, carboxylate stretches are insensitive as to whether saturated or unsaturated carbons are attached to them.

The carbon–oxygen bond order in the $-\text{CO}_2^-$ group is about one and half, and the infrared spectrum shown in Figure 2 will help prove this. A C=O stretch falls at about 1700 (1), and a C–O stretch typically falls at about 1200 (5). Theoretically then a C–O “bond and a half stretch” might fall at the average peak position of these two carbon–oxygen stretching vibrations. The average of 1700 and 1200 is 1450, close to where the carboxylate stretching peaks fall. This close agreement indicates that the carbon–oxygen bond order in carboxylates is approximately 1.5.

Because carboxylates contain positive and negative charges, they are highly polar and have a large dipole moment. Recall from the

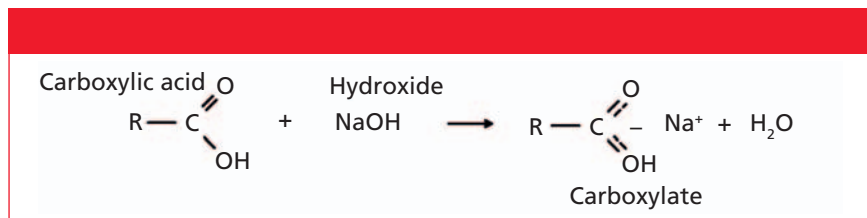


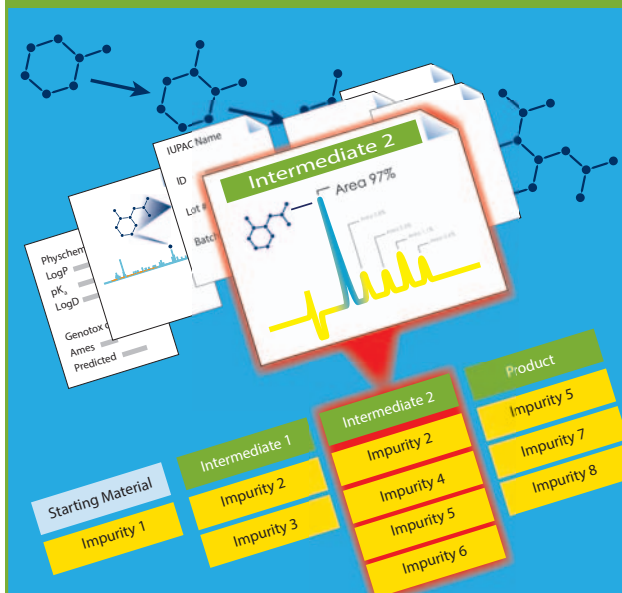
Figure 1: The reaction of a carboxylic acid with sodium hydroxide to give a carboxylate and water.

first installment of this column that one of the characteristics that determine infrared peak positions is the change in dipole moment with respect to bond distance during a vibration, or $d\mu/dx$ (6). When the bonds of the $-\text{CO}_2^-$ group stretch asymmetrically and symmetrically there is a large value of $d\mu/dx$. This attribute is why the pair of carboxylate stretching peaks are so intense.

In theory, one could identify the metal ion in a carboxylate from its mid-infrared spectrum. Recall, however, that as the mass of the atoms in a functional group goes up peak position goes down (7).

Most metal atoms are heavier than the hydrogen, carbon, and oxygen atoms typically found in organic molecules. Thus, the metal–oxygen stretching and bending peaks that might help us determine the metal ion in a carboxylate fall below 400, out of range of most mid-infrared Fourier transform-infrared (FT-IR) spectrometers. Now, carboxylates with different metal atoms will have different infrared spectra because they have different chemical structures (7), but the inability of most FT-IRs to see metal–oxygen peaks makes it difficult to determine the metal ion from the infrared spectrum by itself. In

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

The Last Quiz

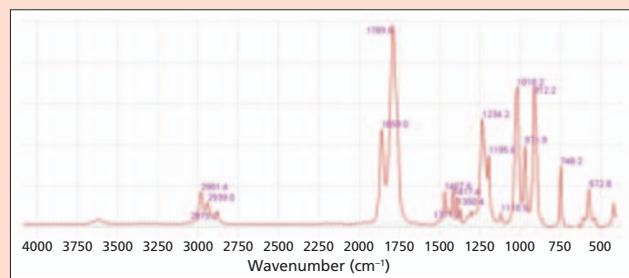


Figure i: The infrared spectrum of 2,2-dimethylsuccinic anhydride ($C_6H_8O_3$), the answer to last installment's quiz.

As we work our way from left to right across the spectrum, the first thing that stands out are the three C-H stretching peaks below 3000, indicating there are CH_2 and CH_3 functional groups present (7). There are no C-H stretches above 3000, so all the carbons present are saturated (7). Looking at these peak positions, 2981 and 2879 can be assigned as methyl asymmetric and symmetric stretches, and 2939 as the asymmetric stretch of a CH_2 group (7). Recall that the ratio of the intensities of the asymmetric CH_2 and CH_3 peaks is sensitive to the CH_2/CH_3 ratio in a sample (7). In Figure *i* the methyl peak is clearly bigger, which means that the CH_2/CH_3 ratio for this sample is less than or equal to 1 (7). The methyl umbrella mode peaks are at 1371 and 1390.

The next major features encountered looking from left to right are the two intense peaks at 1859 and 1789. The intensity and position of these peaks gives them away as C=O stretches (1). The fact that there are a pair of C=O stretches gives this away as an anhydride (4). Because the lower wavenumber peak at 1789 is more intense than the higher wavenumber peak at 1859, this compound is a cyclic anhydride (4). Specifically, 1859 is the symmetric C=O stretch and 1789 is the asymmetric C=O stretch. Since all the carbons are saturated we can conclude that we have a saturated cyclic anhydride. The big peaks at 1234 and 1018 are the C-O stretches of a cyclic anhydride.

The challenge now is determining how many atoms make up the saturated ring in our molecule. Carbon is fond of forming five- and six-membered rings because these are energetically favorable (9). We also know that the CH_2/CH_3 ratio is ≤ 1 , which means there are probably not very many methylenes in the ring. This means the ring more likely has five carbons rather than six. We examined the structure of the five-membered saturated cyclic anhydride succinic anhydride in the last column (4). If we place both methyls on the same carbon, such as is shown in Figure *ii*, we can construct a saturated cyclic anhydride with a CH_2/CH_3 ratio of 0.5, consistent with all we know about this molecule. The structure in Figure *ii* is the answer to the problem, 2,2-dimethylsuccinic anhydride.

Table *i* lists the proper peak assignments for the solution of the problem.

Table i: Peak positions for the problem spectrum from March

2981	1859	1467	1371	912
2939	1789	1417	1234	748
2879	1467	1390	1018	572

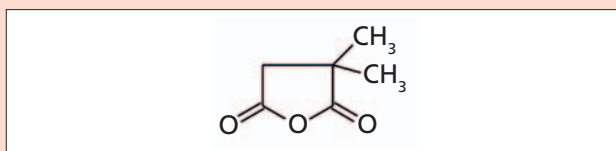


Figure ii: The molecular structure of 2,2-dimethylsuccinic anhydride ($C_6H_8O_3$), the answer to last installment's quiz.

Table ii: The correct peak assignments for last column's problem spectrum.

Peak	Assignment
2981, 2879	CH_3 asymmetric and symmetric stretches
2939	CH_2 asymmetric stretch
1859	Saturated cyclic anhydride symmetric C=O stretch
1789	Saturated cyclic anhydride asymmetric C=O stretch
1390, 1371	CH_3 umbrella modes
1234, 1018	C-O stretches

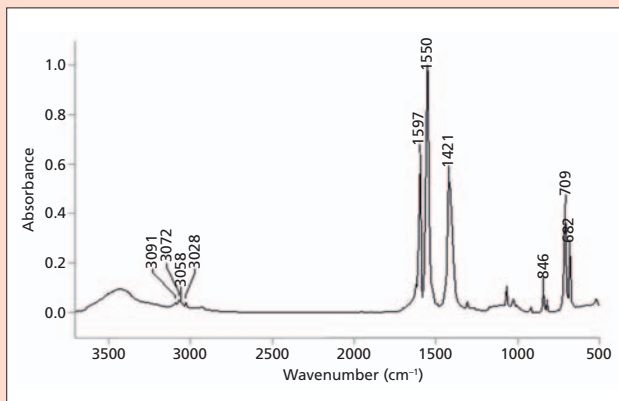


Figure iii: Your next Infrared Spectral Interpretation Workshop challenge.

Table iii: Peak positions for the problem spectrum

3091	3028	1421
3072	1597	709
3058	1550	682

New Quiz

Using everything you have learned in this and previous columns, determine the functional groups present and try to discover the chemical structure of this compound. Remember that inclusion of a peak position in the table does not necessarily mean that it will be useful in the structural determination.

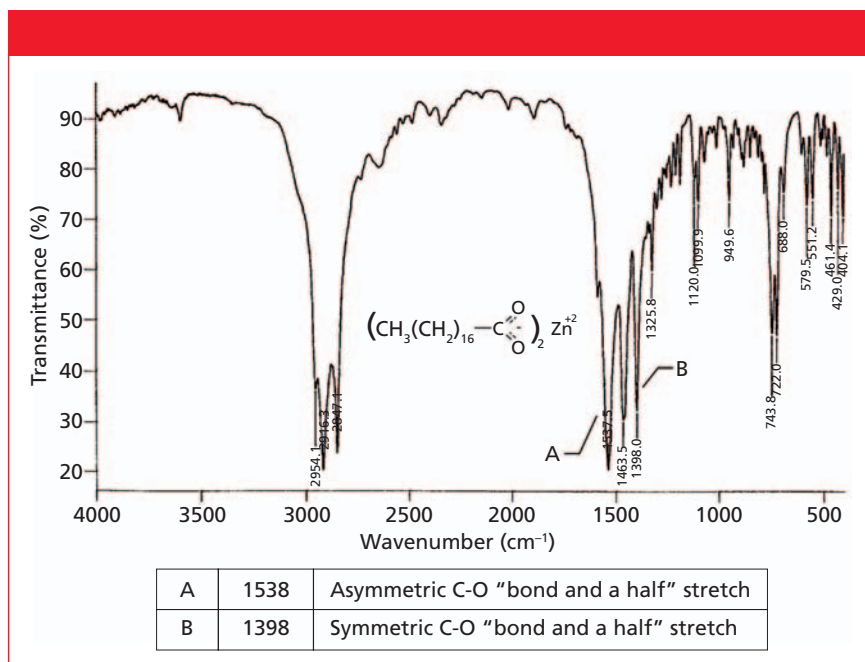


Figure 2: The infrared spectrum of zinc stearate ($C_{36}H_{70}O_4Zn$).

Table 1: The diagnostic infrared group wavenumber for the carboxylate functional group

Vibration	Wavenumber Range
Asymmetric CO_2 stretch	1650–1540
Symmetric CO_2 stretch	1450–1360

this case, consultation of reference spectra, a library search, or a metals analysis of the sample using some form of atomic spectroscopy will be needed.

In the chemical structure of zinc stearate shown in Figure 2 you can see that there are two very long alkyl chains, together whose CH_2/CH_3 ratio is 16. Recall that the relative intensity of the methylene asymmetric stretch compared to the methyl symmetric stretch is proportional to the CH_2/CH_3 ratio for a molecule (7). As can be seen in Figure 2, the CH_2 asymmetric stretching peak at 2916 is significantly larger than the CH_3 asymmetric stretching peak at 2959, as expected.

Also note in Figure 2 that from 1400 down to 400 there are a number of weak to medium intensity peaks. These peaks include C-C stretching bands (8). Under normal circumstances these vibrations

would have small values of $d\mu/dx$, giving difficult to see peaks. Because of the highly polar nature of the carboxylate group, however, the alkyl chain itself is somewhat polarized, which increases $d\mu/dx$ for its vibrations and yields the plethora of peaks seen. The diagnostic group wavenumbers for carboxylates are listed in Table I.

Conclusions

Carboxylates are made by reacting a carboxylic acid with a strong base such as a hydroxide. The structure of the resultant functional group contains a negatively charged $-CO_2^-$ group and a positively charged metal atom, and hence is highly polar. As a result, carboxylates have a large dipole moment and give two intense peaks, assigned as the asymmetric and symmetric $-CO_2^-$ stretches at 1650–1540 and 1450–1360, respectively. The positions of these two peaks indicate that the bond order of $-CO_2^-$ group is about 1.5.

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Brian C. Smith, PhD, has more than three decades of experience as an infrared spectroscopist. He has published numerous peer reviewed papers and has written three books on the subject: *Fundamentals of FTIR and Infrared Spectral Interpretation*, both published by CRC Press, and *Quantitative Spectroscopy: Theory and Practice* published by Elsevier. As a spectroscopic trainer, he has helped thousands of people around the world improve their infrared analyses. He earned his PhD in physical chemistry from Dartmouth College. He can be reached at: SpectroscopyEdit@UBM.com

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Understanding Molecular Interactions with Advanced FT-IR Spectroscopy and Imaging



Advanced vibrational spectroscopic techniques such as Fourier transform infrared (FT-IR) and attenuated total reflection (ATR)-FT-IR spectroscopic imaging are important tools for understanding molecular interactions and using them to help engineer new products and processes. Sergei G. Kazarian of Imperial College London, UK, has used these advanced imaging techniques for applications as varied as studying crude oil fouling, analyzing pharmaceutical formulations in microfluidic channels, examining biological systems and biopsy samples, and investigating the pigment–oil interaction in priceless paintings at the microscale level.

One of your recent publications discusses in situ attenuated total reflection–Fourier transform infrared (ATR-FT-IR) spectroscopic imaging monitoring of asphaltene precipitation from benzene solution and crude oil induced with high-pressure CO₂ (1). What makes ATR-FT-IR imaging a good choice for monitoring this process? What important conclusions were drawn from this research?

Firstly, this research is relevant to understanding crude oil fouling, a problem that has immense economic and energy implications. In this work, we demonstrate an approach of the ATR-FT-IR spectroscopic imaging applied in situ to investigate the stability and behavior of asphaltenes dissolved in different media (benzene and crude oil) at high-pressure CO₂ conditions. The precipitation of asphaltenes from benzene solutions and crude oil induced by high-pressure CO₂ has been studied in situ. This is the first time that the dynamics of precipitation have been observed with ATR-FT-IR spectroscopic imaging, which was used to detect the initial stages of precipitation, to monitor the dynamics of the formation and growth of deposited particles, and to chemically analyze the constituents of the deposits observed under high-pressure conditions.

ATR-FT-IR imaging is the method of choice to study precipitation of asphaltenes because the strong absorption of crude oil in the infrared region makes transmission FT-IR measurements very challenging. ATR-FT-IR spectroscopic imaging probes a thin layer (a few micrometers) of the sample at the bottom

of the high-pressure spectroscopic cell, which provides the unique opportunity to mimic and study the behavior of crude oil at the bottom of the oil container in situ.

It was found that asphaltenes with oxygen-containing functional groups, which are capable of forming specific Lewis acid-base interactions with CO₂, have been observed to precipitate from benzene solution and crude oil at such conditions. Subsequently, based on the obtained spectroscopic data, the mechanism of CO₂-induced precipitation of asphaltenes has been proposed. The obtained results may impact areas as diverse as crude oil production, oil recovery, CO₂ flooding, crude oil fouling, and relevant design or operations by helping oil companies improve their energy efficiency and environmental impact (which ultimately may cut petrol prices). This research is the result of collaboration with Professor O.N. Martyanov at the Boreskov Institute of Catalysis in Novosibirsk, Russia, which celebrates its 60th anniversary this year. Notably, the Society of Applied Spectroscopy, of which I am a Fellow and Editor of its flagship journal, *Applied Spectroscopy*, also celebrates its 60th anniversary.

In a second study (2), you used in situ ATR-FT-IR spectroscopy for imaging pharmaceutical formulations in microfluidic channels to study drug release. What other spectroscopic techniques have been used for this type of study, and what are the advantages of your FT-IR approach over those previous techniques? Microformulations are of significant in-

terest because they can be used to facilitate the development of a wide range of drug delivery systems, including tablet compacts and capsules. The following key question must be answered: How can informative data about multiple microformulations be obtained simultaneously for direct comparison in different microfluidic channels? Recently, a droplet-based microfluidic immunosensor for detection of melamine has been reported that uses a fluorescence polarization method. Ultraviolet (UV) analysis is one method that has shown potential to collect information of drug release in parallel channels using only a few milligrams of the sample. However, no spatial information about the physical or chemical processes occurring within the formulations is revealed and this approach, to date, has not been successfully applied for high-throughput screening approaches. Weitz and coworkers (3) applied fluorescence microscopy to study drug release from microparticles in a microfluidic chip using added dyes, but this approach lacks chemical specificity. However, ATR-FT-IR spectroscopic imaging, an inherently label-free approach, has shown potential for high-throughput screening of static formulations, where spatially resolved information from the different chemical components in the microformulations can be distinguished and structural changes detected, unlike in other approaches. In our macro ATR-FT-IR spectroscopic imaging approach, a combination of three exciting modern technologies was used for the first

time: unique custom designed microfluidic chips; 3D printing technologies (using a microdrop system) for preparing pharmaceutical microformulations; and ATR-FT-IR chemical imaging to understand drug release and dissolution of microformulations. This approach reveals molecular-level insight into the mechanism of dissolution of microformulations and opens a new area of research with direct implications for drug delivery.

A third study in your lab involved mid-infrared spectroscopic imaging of biological systems and biopsy samples. Optical improvements were demonstrated using FT-IR microscopy when conventional sources of infrared radiation were used, as well as application of quantum cascade lasers (QCLs) (4). What challenges were overcome in this study? What are the potential benefits of this approach for clinical analysts?

Indeed, this cited article was largely focused on discussion of optical approaches introduced in my laboratory

for improving the quality of measured FT-IR spectra and the obtained spectroscopic images, as well as discussing the issues of spatial resolution (5). The former discussion includes a demonstration of our pioneering approach with added correcting lenses for removal of chromatic aberration, light scattering, and increased spatial resolution in spectroscopic imaging; this approach was successfully demonstrated in applications to tissues and live cells. The presented examples also demonstrate that the actual achieved spatial resolution in FT-IR imaging is not as high as perceived by researchers using values of theoretical limits or projected pixel sizes.

The use of discrete-frequency QCL approaches, also discussed in this article, provides an opportunity for data reduction without significant loss of achieved classification and also offers a possibility for analysis of much greater areas of samples than were previously feasible using conventional infrared sources. This approach facil-

itates analysis of many samples in a high-throughput manner. We have presented promising preliminary examples of the use of a QCL-based system for obtaining chemical images of esophageal biopsy, but this method can be enhanced further when combined with our correcting lens approach. Recent publications by several other research groups further demonstrate the use of such QCL system for histopathology—for example, by imaging of adenocarcinoma colorectal tissue and high-speed scanning of an entire liver biopsy (6). Furthermore, a very interesting application of QCL for high-throughput analysis of biofluids has recently been demonstrated by Matthew Baker and coworkers (7,8) and by Wrobel and Bhargava for tissue analysis (9), which provides new possibilities for medical diagnosis using such technology. Overall, these spectroscopic methods clearly have the potential to enhance our understanding of chemical changes at an intracellular level and, therefore, pro-

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vide the possibility for the emergence of novel spectroscopic methodologies for enhanced diagnostics.

You have also conducted a study of Jackson Pollock's masterpiece painting *Alchemy*, in which ATR-FT-IR spectroscopic imaging was used for investigation at the microscale level of the pigment–oil interaction in the painting (10). What were the main questions you were attempting to answer in this study?

Yes, this is another exciting application of ATR-FT-IR spectroscopic imaging and I was delighted to collaborate on this research with Italian scientists from Perugia and the Peggy Guggenheim Collection in Venice on spectroscopic studies of microscopic samples from the painting by Jackson Pollock, who is described as one of the greatest figures in the abstract expressionist movement of the 20th century and has produced masterpieces using his unique technique. He routinely used a traditional oil paint (zinc oxide in linseed oil), but was unaware that this type of paint presented a potential threat to the conservation of his paintings. In this work, we applied micro ATR-FT-IR spectroscopic imaging, which we have previously used to study the degradation process of paintings from the National Gallery, London. In this work, we used this approach to detect the mechanism of detrimental formation of zinc soaps occurring inside the painting by Jackson Pollock, thus resulting in its degradation. ATR-FT-IR imaging has helped us to explain that the damage of the painting was related to the formation of zinc soaps around areas where a jellifying agent (aluminum stearate hydroxide) was present that was added in the paint formulation. This finding led to an explanation that this jellifying agent accelerated the formation of zinc soap that usually forms due to the interaction of zinc oxide with fatty acids present in the oil binder of the painting. These chemical processes were reliably assessed due to the high spatial resolution of micro ATR-FT-IR spectroscopic imaging. Previously, we used this spectroscopic approach to analyze a cross-section of hair and live cancer cells, to study atherosclerosis in arterial

tissues, to investigate pharmaceutical tablets, and for many other applications.

This spectroscopic study of Pollock's masterpiece *Alchemy* may help conservation scientists to preserve this, and other, important objects of cultural heritage.

In a very recent study (11), you used ATR-FT-IR spectroscopy to investigate the use of supercritical CO₂ in the processing of polymeric materials in place of organic solvents. What are the advantages and possible disadvantages of using ATR-FT-IR spectroscopy for this application?

This recent article explains why in situ ATR-FT-IR spectroscopy is a powerful method of choice for studies of polymeric materials processed with supercritical CO₂. This approach was pioneered in my laboratory and has since been used by many other researchers in this field. This topic is of significant importance because it has direct implications in CO₂ capture technologies and supporting the drive toward greener solvent alternatives. This article explains why supercritical CO₂ is the method of choice for processing environmentally friendly materials. There are many advantages of using this ATR-FT-IR spectroscopic approach, which include chemical specificity of quantitative in situ analysis by using miniature spectroscopic cells that facilitate the use of a small amount of sample and also make these high-pressure spectroscopic experiments safer.

What are the next steps in your research with infrared spectroscopy?

I expect to continue with other new developments in FT-IR spectroscopic imaging and their application to a broad range of novel research areas. One of our most recent research activities utilizes in situ FT-IR spectroscopy and imaging to understand key processes occurring in chromatographic columns. This work aims to reveal new insights into protein behavior during isolation, so the next steps will be made in this direction and we expect collaboration in this field with biopharmaceutical companies. I would also expect new developments into the design

of new microscopes and spectrometers, such as combining the use of a QCL source with a microscope equipped with added lenses, hemispheres, or an ATR crystal, or both, for greater spatial resolution measurements that would allow the acquisition of higher quality spectroscopic images. These approaches, combined with machine learning techniques, may be applied to cancer diagnosis.

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Review of New Spectroscopic Instrumentation for 2018

Our annual review of products introduced at Pittcon, or during the previous year

Howard Mark and Mike Bradley

Pittcon introduced some significant changes in 2018. The most visible was the decrease in time for the exhibition from four to three days. On Tuesday (the first day), the exhibition floor was very active with what amounted to pent-up energy. However, we must also point out a decrease in the size of the exposition and the absence of some large vendors. There were large seating areas for interactions and even seminars, and the return of the Lab Gauntlet, where vendors present application solutions using their tools. The Gauntlet is a successful addition to the show, with a lot of energy and interest flowing down the aisle. Some presentations (Thermo Fisher Scientific) showed their new products in the Gauntlet, too, making it a continuation, in effect, of booth presentations.

Although Pittcon remains an important venue for the introduction of new products over the past few years, vendors are also increasingly announcing new products outside Pittcon. We therefore accept any new products announced during the past year for inclusion in this review, which covers new instruments, components, and accessories announced by vendors during 2017–2018.

Attendance in 2016 was 12,841 and attendance for 2017 was 14,144. This year's attendance was reported as 11,415 (1). The increase seen last year was attributed mainly to the improving economy. It's not clear whether or not the attendance number reflects only the reduced number of days for the show. Last year we hypothesized that Pittcon attendance might be what economists would call a "lagging indicator."

The exposition featured 714 exhibiting companies occupying 1404 booths, somewhat lower than last year's figure of 787 exhibiting companies. The reduced number of exhibitors might possibly be a result of the reduction of exhibition days to three. Of these companies, 93 were reported as being first-time exhibitors. Increased attendance may persuade more companies to exhibit in the future, as well.

There is a healthy pipeline of new products coming from a wide variety of vendors and application areas. It is good to see continued development around the classic techniques, like near-IR, mid-IR, and Raman spectroscopy. There is a lot of activity around accessories, too, where vendors strive to meet user-specific applications.

For the last couple of years, Pittcon did not present Editor's Choice awards as it had done for many years previously. Last

year, that event was replaced with Pittcon Total Excellence Awards. This year the Excellence Awards seem to have settled down into that new format. The award selection committee consisted of a blue chip panel of experts who evaluated the entries based on "ingenuity, creativity, implementation, and outcomes." Companies are now segregated into small, medium, and large companies based on sales figures so that they can only compete with others in their class. Therefore, there were three awards of each type: gold, silver, and bronze. We are pleased to note that the following spectroscopy companies were winners of the Excellence Awards: In the \$10,000,000–\$100,000,000 sales category, B&W Tek won gold for its STRaman portable Raman analyzer; Metrohm won silver for its 946 Portable VA voltammetric analyzer; and CEM Corporation won bronze for its EDGE extraction system for sample preparation. In the greater than \$100,000,000 sales category, Horiba Scientific won gold for its Duetta fluorescence and absorbance spectrometer (listed in Table III) and Shimadzu Scientific Instruments took home bronze for its IRSpirit FT-IR spectrometer (listed in Table V).

The review that follows is categorized by wavelength region or type of spectroscopy (such as mid-IR, X-ray, and so forth). We arranged our review to allow readers to compare instruments from different manufacturers, although this process sometimes groups handheld instruments with high-end research tools. The categories used to classify the products are

- Accessories
- Atomic spectroscopy
- Components
- Fluorescence
- Mass spectrometry (MS)
- Mid-infrared spectroscopy
- Near-infrared (NIR) spectroscopy
- Nuclear magnetic resonance (NMR)
- Raman spectroscopy
- Software
- UV-visible spectroscopy
- X-ray (includes higher frequencies)

Categories fluctuate from year to year, depending upon trends in the submissions and in the industry. The core spec-

trospectroscopy headings are usually consistent, but marginal categories such as “imaging” have been transient and had no entries this year. Fluorescence has been absent for several years, and we are pleased to see it back as a category. As in the past, “accessories” are tools used in conjunction with an instrument (such as a sample preparation or ATR device), while “components” (such as lasers or detectors) are used within an instrument. The “software” category includes instrument control, collection and data processing programs, as well as products for storage and transmission of data and also collections of data, such as databases (libraries).

Broad Trends

Instrumentation is evolving, like the telephone, to cover a wider array of scientific problems. The high-end instrumentation remains solid, with mainly evolutionary changes: witness the increasing resolution of mass spectrometers. Meanwhile, another trend is reduction in size. For example, routine and field analysis is increasingly being taken over by handheld or portable devices, a trend that seems to be continuing.

The growth we saw in Raman last year continues, with ongoing improvements in the tools and a number of new systems being launched. New generations of small Raman spectrometers continue to appear. Both commercial and academic users of Raman are seeing more laser, detector, and optical options. With this market slated to maintain double-digit growth, we can expect this trend to continue for some time.

Near-IR (NIR) spectroscopy remains a solid method for many analyses, and there is lots of activity in this area. Multiple vendors introduced new tools for NIR, while others have modified existing products to extend their capabilities. The NIR field is not as strong of a growth vector for commercial vendors as Raman. However, it is a core piece of many industrial processes, indicating that we will also see continued developments and improvements in this line.

The largest number of new submissions came from the accessories area. As always, accessories divide generally into sample preparation tools and items

intended for use in probe systems. The key factor, as always, for these vendors has been to recognize a need (like low-cost microtoming) and then devise a targeted tool.

Instruments are also evolving to detect ever-smaller sample sizes. More spectrometers are now reaching the same scales, such as the coupling of Raman and infrared to atomic force microscopes. In addition to microscopes being attached to various optical spectrometers, other couplings

of instruments are starting to appear, such as combined terahertz and FT-IR (mid-IR) spectrometers, and combined mid-IR and Raman in a single unit. The ultimate in small sample size is, of course, the ability to detect and measure the spectrum of a single molecule. We also note that, despite reports from academia about single-molecule detection and characterization, no commercial device has yet appeared in that arena.

Three broad themes emerged from the new products announced to *Spec-*

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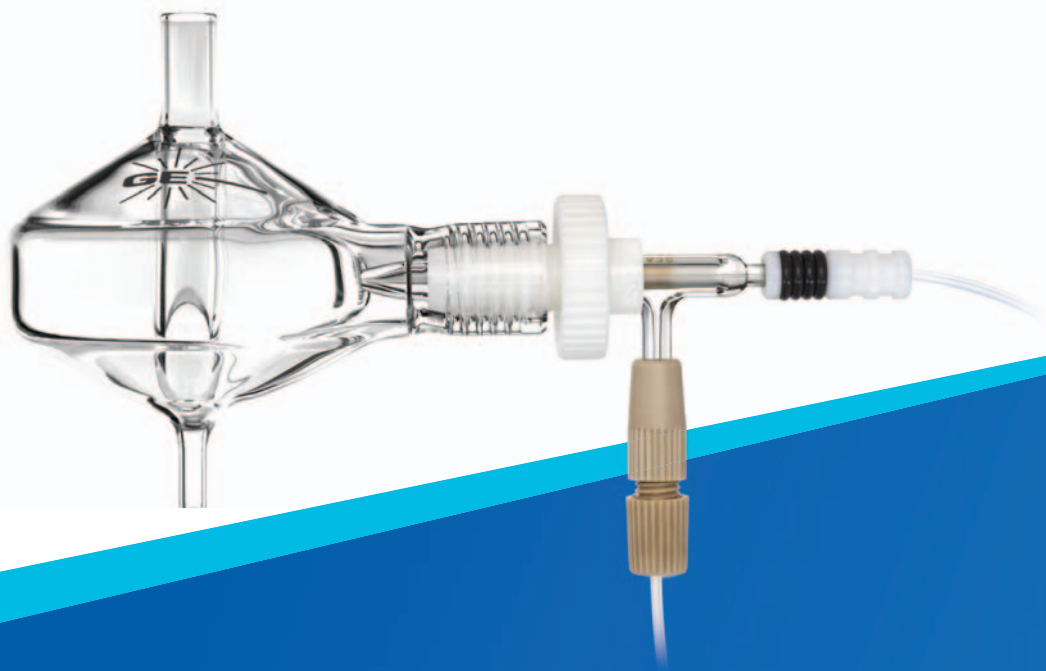
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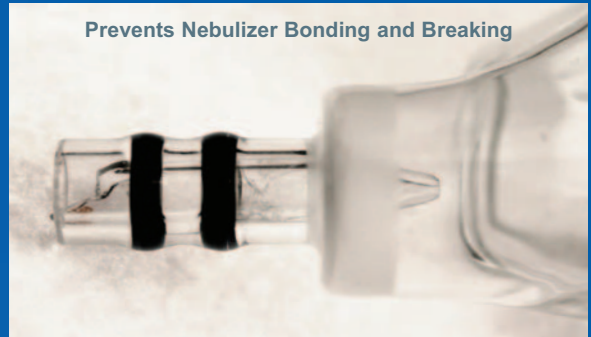
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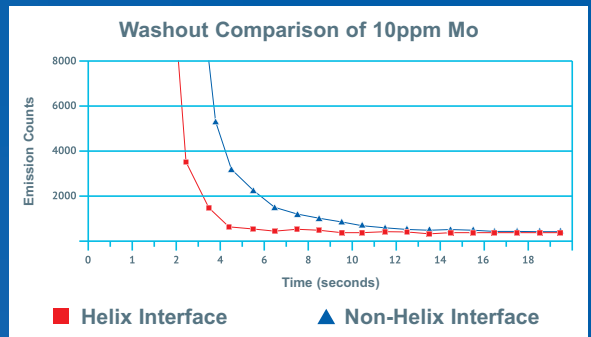
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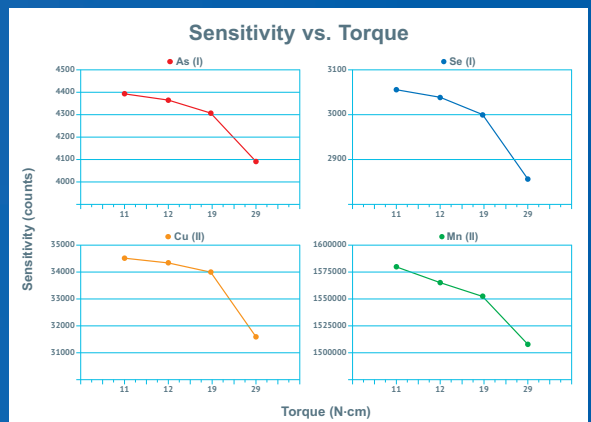


Table I: Index of companies listed in this article

Company Name	Category Listed Under
Advanced Chemistry Development, Inc. (ACD/Labs)	Software
Advion	Accessories
Anton Paar	Accessories and Raman
Avantes	NIR and UV-vis
BaySpec, Inc.	NIR
Bio-Rad Laboratories, Inc.	Software
Block Engineering, LLC	Mid-IR
Brimrose Corporation	NIR
Bruker	Mass spectrometry, mid-IR, NMR and ESR
Cecil Instruments Limited	UV-vis
Cobolt AB	Components
Czitek LLC	Accessories
Eigenvector Research, Inc.	Software
Electro-Optics Technology, Inc.	Components
Energetiq Technology	Components
Excellims Corp.	Mass spectrometry
Fiveash Data Management, Inc.	Software
Galaxy Scientific Inc.	NIR
High-Purity Standards	Accessories
Horiba Scientific	Fluorescence, Raman, software
Ibsen Photonics	UV-vis
JEOL USA	Accessories
JM Science Inc.	Accessories
Laser Components USA, Inc.	Components
LECO Corporation	Atomic
Magritek	NMR and ESR
Malvern Panalytical	X-ray
McPherson	Atomic
Metrohm Raman	Raman
Ondax, Inc.	Accessories
PerkinElmer, Inc.	Atomic, NIR
PicoQuant GmbH	Fluorescence
PIKE Technologies	Accessories
Princeton Instruments	Components
Quantum Analytics	Mid-IR
Saville Corporation	Accessories
Shimadzu Scientific Instruments	Mass spectrometry and mid-IR
Si-Ware Systems	NIR
Specac	Accessories
Spectra Solutions, Inc.	Accessories and Raman
Spectral Engines	NIR
Spectral Evolution	NIR and software
Spectro Analytical Instruments, Inc.	Atomic, X-ray, software
Spectrolight Inc.	Components
Spectrum Scientific, Inc.	Components
ST Japan USA LLC	Accessories
tec5USA	Raman
Thermo Fisher Scientific	Accessories and atomic
TimeGate Instruments	Raman
Wasatch Photonics	Raman, software, UV-vis
Wiley	Software
WITec GmbH	Raman

troscopy and during Pittcon. Classic techniques saw activity. For instance, announcements included multiple tools for the age-old problem of sample preparation (grinding and pressing of samples) and new offerings in inductively coupled plasma (ICP) and FT-IR microscopy. There should be little surprise here—many of the problems faced by today's laboratory workers are the same as those from 20–30 years ago. In spite of exciting developments at the cutting edge, there is plenty of basic chemistry that still needs to be done.

Second, while many vendors are marketing instruments similar to those from years past, the surge in new software developments is continuing. Developments center on two problems: matching the user interface to the problem and lowering sampling barriers. Enlarged databases and new algorithms are combining to provide customized, useful reports. Terrain-following software in microscopy is relieving the problem of focusing on an irregular sample over a large area. And collaboration is being enhanced using video cameras and touch screens to replace single-user eyepieces, allowing local and remote users to tackle problems as a team.

Third, Raman spectroscopy offerings continue to expand. At Pittcon, it seemed every aisle had Raman vendors differentiating their products by size (handheld, portable, or benchtop) and performance. The Raman effect was first observed in 1928, so Raman has had a long development cycle because of some very specific requirements that had to be met to make it a commercially viable technique. The most crucial tool has been the laser, and now many vendors provide multiple diode laser solutions in small packages with low power needs. Vendors can take the ingredients—lasers, miniaturized diffraction elements, and multichannel detectors—and combine them in a particular form factor to address a specific market.

We noted a trend a few years back toward application-specific analyzers. Although this trend seems to have slowed, many vendors have noted how their tools combine in certain markets. See, for example, the new Bruker electron spin resonance beer analyzer, and the

Table II: Atomic spectroscopy products

Company Name	Product Name	Product Type	Measurement Mode	Applications and Unique Features
LECO Corporation	GDS900	UV-vis spectrometer	N/A	Full wavelength coverage from 160 to 460 nm, 50-pm resolution to differentiate complex features of bulk spectra. Glow discharge source gives simple, linear calibrations because controlled excitation occurs away from the sample surface. Cornerstone brand software with touch-screen interface allows for grouping of sample data into sets and replicates to simplify data output and automatically calculate relevant statistics. Optional nitrogen recirculation claimed to reduce nitrogen consumption by more than 1200% annually, and to reduce cost-per-analysis by almost 58%.
McPherson	251MX	Atomic spectrometer	Emission	Flat field and aberration-corrected optics provide better extreme UV and soft X-ray spectra. Narrow symmetrical spectral lines help resolve and discriminate spectral signatures at very short wavelengths. High vacuum housing, optimized coatings, and sensitive cooled CCD detectors with 64-bit software complete the instrument package. Diffraction gratings for 0.5 to 20 nm are complemented by a new low-energy grating. It expands the spectrometers range to 8 eV. All instruments are aligned, tested, and calibrated before shipment.
Perkin-Elmer, Inc.	Avio 500	ICP-OES spectrometer	Emission	A simultaneous, dual-view, compact ICP-OES instrument. It uses a vertical plasma and is engineered to handle difficult, high-matrix samples without dilution. The system is designed to provide high matrix tolerance with a vertical torch design, low argon consumption, simultaneous background correction for fast sample-to-sample time and improved data accuracy, high throughput enabled by dual-view technology, simultaneous data acquisition, and low routine maintenance. Applications: environmental analysis (metals and trace elements in waters and wastes, such as U.S. EPA 200.7, drinking water, and soils); food analysis (toxic and nutritional elements in food samples); pharmaceuticals (elemental impurities in pharmaceutical products according to USP 232/233 and ICH Q3D); lubricants (in-service oil samples in accordance with ASTM D5185 and oil additives in accordance with ASTM D4951); and metallurgical (impurities in metals).

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Table II: Atomic spectroscopy products (continued)				
Company Name	Product Name	Product Type	Measurement Mode	Applications and Unique Features
Perkin-Elmer, Inc.	Nexlon	ICP-MS spectrometer	MS	The NexION 2000 ICP-MS system is designed to allow users to run samples with high total dissolved solids without manual dilution. Its universal cell with three gas channels delivers improved interference removal. Its fast data acquisition speed (100,000 points/s) lets users measure any size particle down to less than 10 nm. New features include an integrated all matrix solution and extended dynamic range capabilities to enable handling of high dissolved solids as well as high- and low-level elements in a single sample; a combination of three gas channels and four modes of operation intended to provide better interference removal for advanced detection limits and provide improved data accuracy; a new solid-state RF generator with LumiCoil technology said to require no maintenance or cooling; and New SmartIntro dedicated sample-introduction modules to simplify operator setup and streamline analytical workflows.
Spectro Analytical Instruments, Inc.	Spectroport	Portable metal analyzer	Optical emission	This portable OES analyzer is designed to deliver advantages of the company's mobile Spectrotest OES analyzer in a smaller, lighter unit, including being designed for effortless point-and-shoot performance; fast, ready response (many analyses take only a few seconds); flexible portability and battery-powered operation; intuitive ease of use; flexible and comprehensive data management; and minimal standardization efforts. Unlike handheld XRF analyzers, it analyzes elements such as carbon, sulfur, phosphorus, boron, lithium, beryllium, calcium, silicon, magnesium, and aluminum at low and critical levels.
	Spectrotest	Mobile metal analyzer	Optical emission	Designed for productivity, reliability, and portability, this analyzer aims to deliver precise results when an exact metal analysis is required, materials are difficult to identify, or there is a large number of samples to be tested. Its high-resolution optical system provides for a wide element range including N, Li, and Na. It provides fast measurements (2 s in sorting mode; from 5 s in analysis mode). Quick, easy-to-change sample probe adapters. Can display results on screen or app, in the laboratory, and onsite.
Thermo Fisher Scientific	iCap	TQ ICP-MS system	ICP-MS	The iCap TQ ICP-MS system is designed to require minimal user maintenance and includes a fully inert sample introduction system, a dry pump for cleanroom environments, and a dedicated gas distribution unit for laboratory safety and maximum flexibility. An ergonomic benchtop design with a compact footprint limits the use of valuable lab space and facilitates integration. It is claimed to provide sub-parts-per-trillion detection, making it an ideal solution for ultraclean applications. The system is designed to retain all the benefits of size and ease of use through streamlined workflows of the existing product line while also providing improved data quality and performance through a combination of cold plasma operation and triple-quadrupole interference removal.

Table III: Fluorescence spectroscopy products				
Company Name	Product Name	Product Type	Measurement Mode	Applications and Unique Features
Horiba Scientific	Duetta	Fluorescence and absorbance spectrometer	Fluorescence, absorbance	The Duetta system can be used as a fluorometer, as a UV-vis-NIR spectrometer to measure absorbance, or to measure true molecular fingerprints, which requires simultaneous acquisition of fluorescence and absorbance, correcting for IFE real time. CCD technology makes it very fast—the system is claimed to be the only fluorometer that can acquire a full spectrum in less than 100 ms. Its CCD technology also extends NIR wavelength detection to 1100 nm, well beyond the limit of standard photomultiplier tube (PMT) fluorometers.
PicoQuant GmbH	FluoTime 300	Fluorescence spectrometer	Fluorescence	A fully automated, high performance fluorescence spectrometer for steady-state, lifetime, and phosphorescence measurements. The FluoTime 300 contains the complete optics and electronics for recording steady-state spectra and fluorescence decays by means of time-correlated single photon counting (TCSPC) or multichannel scaling (MCS) from a few picoseconds to several seconds. The system can be fitted with different kinds of sample holders for most of the applications in that field.

Brimrose Seedmeister NIR analyzer. A new field around cannabinoids is growing. Legalization is opening up new applications in this burgeoning new commodity, which has increased the market for quality control and regula-

tory compliance. This rapidly evolving field historically is populated by high-end instruments—for example, gas chromatography-mass spectrometry (GC-MS)—but now seeking low-cost solutions.

This Year's Products

In each section of the review, every category lists products with a brief synopsis of capabilities as well as a more extensive list of capabilities.

It is always inevitable that some cat-

egories include products that might arguably be classified elsewhere, especially in regard to accessories, components, and software. Some hyphenated techniques, such as inductively coupled plasma–mass spectrometry (ICP-MS) could legitimately be listed in either location. In such cases, the authors usually respected the classification given by the manufacturer.

We also endeavored to provide a synopsis of salient features for each product, or at least as much as could be included in limited space. We follow a “features–benefit” format, so that not only are the key features of a given instrument described, but also the meaningfulness of those features to the user. Also, readers can search by company name or product category in Table I, which references the headings where the content will be found.

Atomic Spectroscopy

This year in the atomic spectroscopy category (Table II), several new ICP instruments with optical emission spectrometry (OES) or MS detection were introduced (PerkinElmer, LECO, and Thermo Fisher Scientific). Like other established methods, the main goals appear to be better detection limits and usability. Spectro Analytical also showed new portable units for the analysis of metals in the field. In recent years, we saw laser-induced breakdown spectroscopy (LIBS) moving in this direction as well.

LECO has full wavelength coverage from 160 to 460 nm, with 50 pm resolution, to differentiate complex features of bulk spectra.

McPherson provides flat field and aberration corrected optics with better extreme UV and soft X-ray spectra. Narrow symmetrical spectral lines help resolve and discriminate spectral signatures at very short wavelengths. The systems include high vacuum housing, optimized coatings, and sensitive cooled charge coupled device (CCD) detectors.

PerkinElmer has the smallest ICP system on the market, with patented Flat Plate plasma technology that uses half the argon of other systems.

Spectro Analytical Instruments has a new advanced, portable OES analyzer

that delivers many of the advantages of the company’s flagship mobile Spectrotest OES analyzer in a smaller, lighter unit.

Fluorescence

Probably the most innovative and exciting development in years for fluorescence (Table III) emerged from Horiba Scientific—an instrument that won best in show at Pittcon. A two-dimensional design allows the Duetta fluorescence and absorbance spectrometer to simultaneously collect—at amazing speeds—UV–vis–NIR absorbance spectra at the same time as the fluorescence is captured. This device should prove to be valuable in drug discovery laboratories and related fields in biophysics. A second new instrument, from PicoQuant, provides access to steady-state, lifetime, and phosphorescence.

Horiba’s instrument can measure fluorescence and UV–vis absorbance spectra, and can also do both simultaneously

PicoQuant shows its FluoTime 300 fully automated, high-performance fluorescence spectrometer for steady-state, lifetime, and phosphorescence measurements.

Mass Spectrometry

A few new products were introduced in the MS category (Table IV) this year. For example, Shimadzu, introduced a matrix-assisted laser desorption–ionization time-of-flight (MALDI-TOF) front-end designed for efficient sample introduction.

Bruker Daltonik offers a TOF mass spectrometer specialized to improve the analysis of the proteome.

Excellims shows a compact ion mobility analyzer for analytical laboratories and at-line applications. Combining high resolution ($R > 70$) and soft electrospray ionization to allow for the introduction of a wide range of compounds, the GA2200 analyzer permits chemical analysis of mixtures in seconds.

Shimadzu provides a benchtop TOF mass spectrometer that improves laboratory efficiency and accelerates analysis through a newly designed load–lock system for rapid sample target introduction and a solid-state laser for fast data acquisition speeds.



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Table IV: Mass spectrometry products				
Company Name	Product Name	Product Type	Measurement Mode	Applications and Unique Features
Bruker Daltonik GmbH	timsTOF Pro	Mass spectrometer	Mass spectrometry	The timsTOF Pro system is designed to dig deeper into the proteome. With the PASEF method, the MS/MS spectra quality of low-abundance peptides can be increased by selecting them several times. Peptide mixtures are still extremely complex when analyzed in two dimensions (retention time and m/z); therefore, by adding another dimension, scientists in the field of shotgun proteomics do not have to choose a trade-off between resolution, scan speed, and sensitivity.
Excellims Corp.	GA2200	Stand-alone high performance ion mobility mass spectrometer	Mass spectrometry	A compact ion mobility analyzer for analytical laboratories and at-line applications. Combining high resolution ($R > 70$) and soft electrospray ionization to allow for the introduction of a wide range of compounds, the system permits chemical analysis of mixtures in seconds. Building on the GA2100, the GA2200 offers an improved electrospray source that permits the direct analysis of individual syringes, continuous flow connection to autosamplers or LC instruments, and gas analysis without having to change sources.
Shimadzu Scientific Instruments	MALDI-8020	MALDI-TOF mass spectrometer	Mass spectrometry	The benchtop MALDI-8020 MS system is designed to improve laboratory efficiency and accelerate analysis through a newly designed load-lock system for rapid sample target introduction and a solid-state laser for fast data acquisition speeds. Design features include automated source cleaning and an integrated barcode scanner to improve workflows and facilitate routine maintenance. The user interface enables 21 CFR Part 11 compliance to make it suitable for both regulated and research environments. Applications: analysis of proteins, peptides, and polymers in academia.

Table V: Mid-IR products				
Company Name	Product Name	Product Type	Measurement Mode	Applications and Unique Features
Block Engineering, LLC	LaserWarn	Mid-IR spectrometer	Open path	Uses open-path chemical detection and simultaneously offers detection of large number of chemicals (hundreds or even thousands), as a result of the use of ultrawidely tunable quantum cascade lasers and new class of detection algorithms; long paths (500 m) for large area coverage; compact optics (2–3 in.) for ease of installation; a long lifetime (no moving parts, all solid-state components); and no consumables for minimal maintenance.
Bruker Optik GmbH	Invenio	FT-IR gas analyzer	Transmission, specular and diffuse reflectance, ATR, emission	This system is a multispectral range FT-IR research and development spectrometer that allows for up to seven internal software-controlled detectors. A unique additional transit channel allows for mid-IR transmittance measurements without removing research setups from the main sample compartment. The optional integrated touch panel enables an intuitive workflow. Bruker FM technology is designed to allow for simultaneous mid- and far-infrared spectroscopy. The optics bench delivers high throughput with a footprint optimized for laboratory benches.
Quantum Analytics	IRmadillo	FT-IR spectrometer	ATR	A solid-state instrument certified for use in hazardous and explosive environments. It can be mounted directly on, or in-line with, manufacturing vessels, and is designed to excel at continuous monitoring of industrial liquids and slurries. Impervious to vibration, this in situ sensor monitors reactions live, and tells the analyst what reactions are doing as they occur. No more need to wait for analysis results to return from remote sampling techniques such as with HPLC or GC.
Shimadzu Scientific Instruments	IRSpirit	FT-IR spectrophotometer	Transmission	Small and lightweight, this spectrophotometer is intended to provide unmatched functionality in its class of compact instruments with a design that allows access from a standard-sized sample compartment that accommodates a wide range of existing accessories. A dedicated analysis assistant program gives analysts the ability to measure samples or print results with a few mouse clicks. In addition, the program is designed to allow operators with minimal experience to obtain results quickly.

Mid-IR

In mid-IR (Table V), three different approaches to the infrared analysis of materials are reported in this year's new developments. Quantum cascade lasers continue to appear in new configurations. The crowded field of small bench-

top instruments saw new and refreshed instruments from Shimadzu Scientific Instruments and Bruker Daltonik, respectively. And a solid-state instrument designed for hazardous environments was introduced by Quantum Analytics.

Block Engineering has configured

QC lasers for a breakthrough in open-path chemical detection and measurement that simultaneously offers detection of large numbers of chemicals (hundreds or even thousands), resulting from the use of world-record, ultrawidely tunable quantum cascade

lasers, and a new class of sophisticated detection algorithms.

Bruker offers a multispectral range FT-IR R&D spectrometer with many innovative features, including detector technology that allows for up to seven internal software-controlled detectors. A unique additional channel allows for mid-IR transmittance measurements without removing research setups from the main sample compartment.

Quantum Analytics has introduced a solid-state instrument certified for use in hazardous and explosive environments. It is mounted directly on, or in-line with, manufacturing vessels, and excels at continuous monitoring of industrial liquids and slurries. Impervious to vibration, this in situ sensor monitors reactions live.

Shimadzu Scientific Instruments provides unmatched functionality in its class of compact instruments with a design that allows access and a standard-sized sample compartment that accommodates a wide range of existing accessories.

NIR

This year, there was a lot of activity around NIR instrumentation (Table VI). Portability was a major theme of offerings from companies such as BaySpec, Spectral Evolution, and Spectral Engines. Food-targeted analyzers were also developed by Brimrose and Avantes, showing that the analyzer theme seen some years back continues in the NIR space, but at a slowed pace. Adaptation of existing equipment into the NIR space was also shown by PerkinElmer.

Another general trend that started off slowly a while back and seems to be continuing is for manufacturers to provide instruments precalibrated for the commodities (and the analytes in those commodities) that their customers want to measure.

Avantes has new and improved versions of NIR spectrometers that are based on a 100-mm optical bench with a numerical aperture (NA) of 0.13 that offer an optimal balance between resolution and sensitivity. The 2.5-HSC series spectrometers feature 256- or 512-pixel InGaAs detectors and are available in multiple configurations.

Bayspec has the world's smartest palm spectrometer, the Breeze spectrometer for the 400–1700 nm range. Featuring proprietary miniaturized optics, the spectrometer is highly efficient for maximum sensitivity with ultrafast acquisition.

The Brimrose Seedmeister Mark III acousto-optic tunable filter (AOTF)-NIR spectrometer is focused specifically on the comprehensive understanding of peanuts. The unit is able through nondestructive testing to fully characterize such properties as protein, moisture, starch, oleic, and linoleic oils.

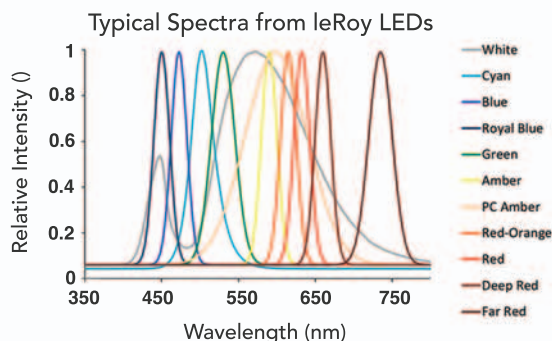
The Galaxy QuasIR 1000 NIR spectrometer ensures direct calibration transfer without the frustration of standardizing instruments or adjusting models to accommodate excessive instrument variability. Edible oils, lubricants, and fuels can be easily analyzed for quality control or adulteration.

PerkinElmer's Spectrum Two N spectrometer is a high-performance, robust, and transportable FT-NIR system platform enabling simple, reliable NIR analyses, ideal for laboratories that need to combine high-end performance with the ease-of-use features of a portable instrument.

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Table VI: NIR products				
Company Name	Product Name	Product Type	Measurement Mode	Applications and Unique Features
Avantes	AvaSpec-NIR256/512-2.5-HSC-EVO	NIR spectrometer	N/A	The new and improved versions of the Avantes NIR spectrometers are based on a 100-mm optical bench with NA of 0.13 to offer balance between resolution and sensitivity. The 2.5-HSC series features 256- or 512-pixel InGaAs detectors, and they are available in multiple configurations. The 256-pixel detectors offer the best sensitivity for most applications.
BaySpec, Inc.	Breeze	Palm NIR spectrometer	Transmission, reflection	Breeze is a palm-sized spectrometer for 400–1700 nm measurements. It features miniaturized optics and is designed to be highly efficient for maximum sensitivity with ultrafast acquisition. This device is designed to deliver laboratory performance with one-touch-of-a-button operation. It allows for wireless communication to any smartphone via a Bluetooth interface. With an available data library, this device can perform quantitative and qualitative analysis at any time and anywhere.
Brimrose Corporation	Seedmeister	NIR spectrometer	AOTF diffuse reflectance	The Brimrose Seedmeister Mark III AOTF-NIR spectrometer is focused specifically on the comprehensive understanding of peanuts. The unit is able, through nondestructive testing, to fully characterize properties such as protein, moisture, starch, and oleic and linoleic oils. The spectrometer is designed to be accurate, repeatable, and low cost. It is an updated version of the Seedmeister Luminar 3076. This unit can scan seeds of all peanut sizes.
Galaxy Scientific Inc.	QuasIR 4000	Transmission and integrating sphere FT-NIR spectrometer	Transmission, diffuse reflection	The QuasIR 4000 spectrometer was designed to offer NIR analysis that combines portability and high spectroscopic performance for fast, accurate results. It is designed to ensure direct calibration transfer without standardizing instruments or adjusting models to accommodate excessive instrument variability. New this year: a temperature controlled transmission cell; both a standard integrating sphere for reflectance measurements and a transmission cell capable of holding a cuvette or a vial; and thermoelectric temperature control to provide the stability and temperature range to precisely measure transmission samples such as edible oils, lubricants, and fuels.
Perkin-Elmer, Inc.	Spectrum Two N	FT-NIR spectrometer	NIR spectroscopy	A high-performance, robust, and transportable FT-NIR system platform designed to enable simple, reliable NIR analyses. Designed for laboratories that need to combine high-end performance with the ease-of-use features of a portable instrument, to allow users with different levels of expertise to be proficient with it quickly. A flexible design with optimized “plug-and-play” sampling and analysis modules helps ensure the best solution for a range of qualitative, quantitative, and adulterant screening applications.
Si-Ware Systems	NeoSpectra Micro Spectral Sensor	FT-IR spectral sensors	Reflection, transmission	These compact, low-cost FT-NIR spectral sensors are designed for quantification, qualification, or identification. Sensors are constructed from components designed to be robust, permanently aligned, and highly reproducible. Core technology is based on microelectromechanical systems (MEMS) technology. The NeoSpectra Micro is the second-generation spectral sensor from NeoSpectra. It is just as accurate, scaleable, and robust as its predecessor, but it has been miniaturized to only 10 mm x 10 mm. The NeoSpectra Micro is designed for use in quantitative and qualitative material analysis in a wide range of application areas in industrial or consumer environments. It is designed to be easily integrated into value-added systems for agriculture, food, pharmaceuticals, oil and gas, polymers, and biotechnology.
Spectral Engines	NIRone Scanner	Scanner	N/A	This battery-powered scanner pairs wireless and Bluetooth connectivity with the NIRone NIR sensor and light sources from Spectral Engines.
	NIRone Sensor	Sensor	N/A	This sensor incorporates a Fabry-Perot MEMS sensor and light sources. It is designed to provide a large dynamic range and stability in the face of temperature changes and vibration. The typical signal-to-noise ratio is >10,000 for a single measurement. Onboard I2C and UART communication, plus a digital trigger, make the sensor ready for OEM integration.
Spectral Evolution	PSR-1100f	Spectroradiometer	Transmission, reflection	Spectral Evolution’s smallest, lightest, full-featured field spectroradiometer with a spectral range of 320–1100 nm. It can be used with a laptop or handheld microcomputer, or as a stand-alone instrument with its built-in keypad and liquid crystal display. It provides a 25°, 1-m fiber optic cable with industry-standard FC connections and allows users to select from 1, 2, 3, 4, 5, 8, and 10° field of view lenses, or to connect to a handheld contact probe or a leaf clip.
	SR-6500	Spectroradiometer	Transmission, reflection	The SR-6500 spectroradiometer claims to offer the highest resolution and highest sensitivity available in a field-portable system. Resolution at FWHM is 1.5 nm at 700 nm, 3.0 nm at 1500 nm, and 3.8 nm at 2100 nm. It features the following noise equivalence radiance (NER) performance with a 1.5-m fiber optic: 0.8×10^{-9} W/cm ² /nm/sr at 400 nm, 0.3×10^{-9} W/cm ² /nm/sr at 1500 nm, and 5.8×10^{-9} W/cm ² /nm/sr at 2100 nm. The system is ideal for remote sensing applications.

Table VII: NMR and ESR products				
Company Name	Product Name	Product Type	Measurement Mode	Applications and Unique Features
Bruker BioSpin	The Beer Freshness Package	microESR	ESR	The Beer Freshness solution is the result of a collaboration between Bruker and FlavorActiv. The solution, which consists of an ESR instrument and custom software, aims to optimize brewing operations and storage conditions to provide maximum antioxidant content in packaged beer. This information allows manufacturers to enhance their production process by taking corrective action earlier in the process, helping to ensure product freshness and stability.
Magritek	Spinsolve 80	NMR spectrometer	NMR	A multinuclear NMR spectrometer with 80-MHz field strength designed to deliver unrivaled power and the best performance of any benchtop NMR system. It has a small footprint and low weight. The spectrometer is the newest product in Magritek's Spinsolve family. It is designed to maintain high performance and quality standards. The spectrometer can perform even the advanced multinuclear methods, such as COSY, DEPT, HSQC-ME, and HMBC, with a single click.
	Spinsolve Ultra	NMR spectrometer	NMR	The Spinsolve Ultra benchtop NMR spectrometer offers enhanced resolution (50% < 0.2 Hz) combined with solvent suppression to expand the range of benchtop NMR applications to ones where submillimolar concentrations of substances can be quantified in the presence of neat protonated solvents in less than 8 min. Advances in the shimming technology of Magritek's high homogeneity Halbach magnets make the spectrometer the company's most versatile benchtop NMR system. The spectrometer is capable of resolving small NMR signals in the presence of large solvent signals.

Si-Ware Systems provides a compact, low-cost FT-IR spectral sensor that delivers the spectral response of the light absorbed by materials for quantification, qualification, or identification.

Spectral Engines provides an NIR sensor that incorporates a Fabry-Perot microelectromechanical systems (MEMS) sensor and light sources. The NIRone NIR sensor has a large dynamic range and stability in the face of temperature changes and vibration, and also offers a battery-powered scanner that pairs wireless and Bluetooth connectivity with the NIRone NIR sensor and light sources.

Spectral Evolution has its smallest, lightest, full-featured field spectroradiometer that has a spectral range of 320–1100 nm and can be used with a laptop or handheld microcomputer, or as a standalone instrument with its built-in keypad and liquid crystal display (LCD). It provides a 25°, 1-m fiber-optic cable with industry-standard FC connections and allows users to select from 1, 2, 3, 4, 5, 8, and 10° field of view lenses or connect to a handheld contact probe or unique leaf clip.

NMR and ESR

Only one manufacturer, Magritek, showed new instrumentation, continuing to develop the benchtop NMR area. This area (Table VII) continues to show increasing promise as the fields increase, improving sensitivity and providing access to more nuclei. There are also related developments in NMR–electron spin resonance (ESR) methods applied to specific markets.

Bruker's Beer Freshness solution, consisting of an ESR instrument with custom software and database, is the result of a collaboration between Bruker and FlavorActiv. The solution aims to optimize brewing operations and storage conditions to provide maximum antioxidant content in packaged beer.

Magritek has a carbon benchtop NMR spectrometer that provides remarkable 60-MHz NMR performance in a compact, benchtop instrument including 1D and 2D NMR experiment capability, with ^1H , ^{19}F , and ^{13}C nuclei.

Raman

Recent trade shows like Pittcon have seen many new Raman systems being shown (Table VIII). While fewer new devices appeared this year, there were innovations, especially around small scale and original equipment manufacturer (OEM) instruments. The most unusual entrant this year, from TimeGate Instruments, strives to eliminate the old enemy of Raman—

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Table VIII: Raman products				
Company Name	Product Name	Product Type	Measurement Mode	Applications and Unique Features
Anton Paar	Cora 5X00	Raman spectrometer	Raman scattering	A compact, benchtop Raman platform that integrates a volume phase grating (VPG) for high light throughput to obtain fast, accurate analysis with multiple laser wavelengths to help eliminate fluorescence interference. Users can choose between 532-, 785-, and 1064-nm wavelengths as well as a variety of sample holders or fiber probes.
Horiba Scientific	Anywhere Raman	Gemstones identification system	Reflection	The AnywhereRaman system is self-contained instrument combining a spectrometer, a laser, and an acquisition computer that fiber-optically couples to a Raman ball probe to obtain high-quality Raman measurements without multiple boxes or need to focus. It is designed for both portability and ease of use, requiring minimal training or experience. The ball probe with TouchRaman immersion technology lets users simply touch the sample and acquire data.
Metrohm Raman	Mira DS (Metrohm Instant Raman Analyzer—Defense and Security)	Raman spectrometer	Raman scattering	This small handheld Raman analyzer is designed to bring the precision of laboratory analysis to first responders in the field. Automated data collection, combined with a comprehensive library of illicit materials and advanced mixture matching routines, provides defense and security professionals with immediate information about potential threats. Safety features designed to provide users with actionable intelligence include ruggedization, choice of attachments for sampling flexibility, remote and delayed acquisition, and color-coded hazard warnings.
Spectra Solutions, Inc.	Raman process instrument	Raman spectrometer	Raman scattering	The key features of the Raman process instrument are a high throughput spectrograph with multifiber input and thermoelectrically cooled CCD ($-60\text{ }^{\circ}\text{C}$), and ability to monitor up to six probes simultaneously. Each probe is connected to its own laser source and rack mountable instrument housing. Available with 532-, 671-, and 785-nm lasers. Spectral acquisition software allows integration of Matlab and Eigenvector Solo Predictor Engine for chemometric analysis and process monitoring.
	Raman spectrograph	Raman spectrometer	Raman scattering	The key features of the Raman spectrographs include an F2 optics high-throughput volume phase holographic grating, two-dimensional CCD detector with thermoelectric cooling to $-60\text{ }^{\circ}\text{C}$, single or multiple-fiber input for simultaneous measurements of multiple probes, compact size, and no moving parts. Available in 785-, 671-, and 532-nm Raman versions. Average resolution is 8 cm^{-1} for a $50\text{-}\mu\text{m}$ slit and 4 cm^{-1} for a $25\text{-}\mu\text{m}$ slit.
tec5USA	MUX-piezo for Raman	Raman spectrometer	Raman scattering	The tec5USA MultiSpec Raman spectrometer is a versatile platform for laboratory and process measurements. It features a 785-nm laser (class 3B) tunable from 50 to 500 mW, and a thermoelectrically cooled high-resolution CCD detector.
TimeGate Instruments	TimeGate PicoRaman	Raman spectrometer	Raman scattering	The PicoRaman spectrometer minimizes or eliminates background sample fluorescence using a combination of a picosecond laser and picosecond detector. The Raman scattering from the pulsed laser is prompt, and the fluorescence, which is delayed, is gated out by the ultrafast detector.
Wasatch Photonics	WP 785	OEM Raman spectrometer series	Raman scattering	Drop-in OEM modules deliver high performance Raman in a robust, compact package. The transmission VPH grating design uses diffraction-limited optics in a high efficiency f/1.3 optical bench to deliver measurement speed and limit of detection comparable to laboratory systems. Excellent unit-to-unit repeatability and temperature stability facilitate library matching for better, more dependable answers. Available as fiber-coupled, free space, or integrated laser models with choice of detector cooling (ambient, regulated, or thermoelectrically cooled).
WITec GmbH	WITec Active Focus Stabilization	Active Focus Stabilization	N/A	A new feature of the recently released WITec Suite V operating software. Confocal Raman microscopy investigations performed on delicate samples often require lower excitation power and a corresponding increase in acquisition time. Active focus stabilization optimizes the Raman signal by ensuring that the focus between the microscope objective and sample is maintained and signal collection is unaffected while temperature or humidity changes.

fluorescence—through time gating of the signal.

Anton Paar has a compact, benchtop Raman platform that integrates a volume phase grating for high light throughput.

Horiba Scientific manufactures and combines a spectrometer, laser, and acquisition computer in one instrument that fiber-optically couples to a Raman ball probe to obtain

high-quality Raman measurements without multiple boxes or need to focus.

Metrohm shows the smallest handheld Raman analyzer available, designed to

bring the precision of laboratory analysis to first responders in the field.

Raman process instruments from Spectra Solutions include a high-throughput spectrograph with multifiber input and thermoelectrically cooled CCD (-60 °C) and can monitor up to six different probes simultaneously. Each probe is connected to its own laser source and rack-mountable instrument housing.

The tec5USA MultiSpec Raman system is a versatile platform for laboratory and process measurements. It features a 785-nm laser (class 3B) variable from 50 to 500 mW, and a thermoelectrically cooled high-resolution CCD detector.

Timegate Instruments eliminates background sample fluorescence using a combination of a picosecond laser and picosecond detector. The Raman scattering from the pulsed laser is prompt, and the fluorescence, which is delayed, is gated out by the ultrafast detector.

Wasatch Photonics offers a drop-in OEM module that delivers high-performance Raman spectroscopy in a robust, compact package.

WITec's Active Stabilization software feature optimizes the Raman signal by ensuring that the focus between the microscope objective and sample is maintained, even in the face of changes in the environment.

UV-vis

UV-vis instruments (Table IX) are workhorses in the analytical laboratory. With a long history of applications and new ones arising—especially in the pharmaceutical world—many vendors continue to develop these tools. The improvements center around speed of the analysis, decreasing the sample size, and increasing the sensitivity in a smaller instrument.

Avantes presents two new instruments, the Hero and the MKII UV-vis spectrometers. The former instrument emphasizes spectral sensitivity, and the latter features a detector array with more pixels for better spatial resolution.

Cecil Instruments has a double-beam instrument that can perform preprogrammed assays.

Ibsen's Freedom C spectrometer introduces a new 4096px detector that enables higher resolution for the UV region down to 0.15 nm.

Wasatch Photonics has a new UV-vis spectrometer series that delivers analytical laboratory-grade performance in a compact footprint. Its proprietary transmission volume phase holographic grating design maximizes efficiency and reduces stray light to extremely low levels.

X-ray

Both companies in this section of the review introduce X-ray equipment (Table X) that stresses small spot sizes and speed of response.

Malvern Panalytical (formerly Malvern) supplies the Epsilon 1 analyzer for small-spot X-ray analysis, which offers users the capability to analyze samples with a 1-mm measurement spot.

The Midex MID05 energy dispersive X-ray fluorescence spectrometer from Spectro Analytical Instruments is designed to provide exceptional performance, high precision, and accuracy for a wide range of precious metal alloys, with testing times as low as 15 s, for more than 30 elements backed by extensive factory calibrations.

Software

Software (Table XI) consists of several different, albeit related, types of products. The first, and arguably the main type, is actual computer programs (that is, the sequences of instructions computers use to carry out their functions).

A large number of new software products appeared this year. The software interface and the attainment of results are now the core of user experience. Clearly, helping users move rapidly from a sample to a result is becoming a major goal of both instrument developers and pure software companies. There is also movement in the area of spectral libraries (vibrational and MS), as new materials and new demands are causing the industry to reach for new reference standards to hit customer targets.

The second type of product consists of collections of various types of data. One important subcategory of this product type consists of actual databases—sets of related data that can be used in a manner similar to dictio-

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Table IX: UV–vis spectroscopy products

Company Name	Product Name	Product Type	Measurement Mode	Applications and Unique Features
Avantes	AvaSpec-Hero	UV–vis spectrometer	Transmission	Designed for high resolution and high sensitivity, the AvaSpec-Hero is built up around the company's high sensitivity compact 100-m optical bench and offers a numerical aperture (NA) of 0.13 and a cooled backthinned detector (1024 x 58 pixels). For the electronics, the newest AS7010 board is used including a high performance analog-to-digital converter with excellent noise performance and the ability to communicate at a high speed through USB 3.0 and Ethernet. The instrument is designed to offer balance between sensitivity and resolution, and the capability of using longer integration times in low-light applications without compromising signal-to-noise performance. The spectrometer is designed for use with replaceable slits.
	AvaSpec-mini MKII	UV–vis spectrometer	Transmission	The AvaSpec-Mini-CL series can be equipped with a 2048-pixel CMOS detector or a 4096-pixel array. They are designed to provide the speed and enhanced native UV–NIR response of CMOS with resolution to 0.1 nm. The low stray-light design allows less than 0.2% stray light, and it is capable of data transfer speeds as fast as 4.6 ms/scan and integrations times ranging from 30 μ s to 59 s. The new AvaSpec-Mini-MK-II includes a CMOS detector and a 4096-pixel array. The company says it ensures unit-to-unit reproducibility and excellent temperature stability.
Cecil Instruments Limited	BioAquarius	UV–vis spectrometer	Double beam	The double-beam BioAquarius spectrometer performs preprogrammed assays for nucleic acids, proteins, oligonucleotides, experimental thermal melt, kinetics, and cell-culture determinations. This spectrometer may be used for any UV–vis spectrometer laboratory task. It may be used with a wide range of accessories, including proprietary third-party nano cells. DataStream software provides PC control and PC storage of data.
Ibsen Photonics	Freedom HR	Vis–NIR spectrometer	N/A	The Freedom HR spectrometer offers a balance between compact size and high performance as a result of the use of unique transmission grating technology. This robust, athermal, industrial-grade diode array-based spectrometer can operate under demanding environmental conditions. The spectrometer supports many different detector systems, which enables users to choose the best detector option for a specific application.
Wasatch Photonics	WP UV–vis	Spectrometer series	Absorbance, transmission, reflection	This UV–vis spectrometer series delivers laboratory-grade performance in a compact footprint. A proprietary transmission VPH grating design maximizes efficiency and reduces stray light to extremely low levels. This facilitates fast data sampling rates and very low limit of detection. Absorbance measurements at 300 nm are linear up to 3.7 AU—comparable to larger, expensive spectrophotometers. The spectrometer covers 250–850 nm, with multiple detector options to match application and budget.

Table X: X-ray spectroscopy products

Company Name	Product Name	Product Type	Measurement Mode	Applications and Unique Features
Malvern Panalytical	Epsilon-1	Small-spot analysis	Reflection	The Epsilon 1 system for small spot analysis offers users the capability to analyze detail samples with a 1-mm measurement spot. It is equipped with standardless software and is available for a wide range of applications. It is possible to comply with ASTM F2617 test method for RoHS-2 analysis, in combination with the 1-mm spot. This version of the system is equipped with a camera and a 1-mm measurement spot, and it has 15-W excitation capabilities. Applications: RoHS-2 analysis (compliant with ASTM F2617), jewelry, toys, ceramics, geology, forensics, manufacturing.
Spectro Analytical Instruments, Inc.	Spectro Midex MID05	Small-Spot ED-XRF spectrometer for precious metal testing	X-ray fluorescence	This ED-XRF system is designed to provide exceptional performance and high precision and accuracy for a wide range of precious metal alloys. It is said to provide testing times low as 15 s and can analyze >30 elements backed by extensive factory calibrations with accuracy for traces and majors. It is designed for high reliability, cost-effective analysis, and ease of use for minimally trained operators.

naries or encyclopedias (as compendia of important facts and relationships among those facts).

A third type of product that we would include under the heading of

“software” is somewhat unique to the fact that spectroscopy is heavily dependent on chemometric algorithms. This software, therefore, consists of the models, or collections of models (that

is, a “database” of models) that can be used by the chemometrics algorithms to analyze future samples. This category tends to be promoted by instrument manufacturers to further their

Table XI: Software products

Company Name	Product Name	Product Type	Applications and Unique Features
Advanced Chemistry Development, Inc. (ACD/Labs)	Luminata	Informatics software	Luminata is an informatics system that enables organizations to establish effective impurity control strategies based on assembled chromatographic, analytical, and chemical information in a single environment. The software facilitates assembly of live, multitechnique analytical and chromatographic data, no matter the instrument vendor, with related chemical entities. Automated data processing and analysis reduces the need for data transcription and interactivity facilitates collaboration in multidisciplinary project teams with up-to-date information.
Bio-Rad Laboratories, Inc.	KnowItAll Informatics System 2018	Spectroscopy software and spectral libraries	KnowItAll software offers integrated solutions to analyze and manage multiple types of spectra (IR, NMR, NIR, MS, Raman, UV-vis, and chromatograms) in multiple instrument formats. It includes patented tools not available in other spectroscopy packages. Combined with a large spectral reference database, the software is designed to give chemists the advanced technology for fast, accurate results. KnowItAll 2018 is a spectral library collection of more than 2.5 million spectra. Advanced stereochemistry recognition has also been added to the ChemWindow application that's included with the software.
Eigenvector Research, Inc.	Solo	Stand-alone chemometrics software	Tools include PLS, PCA, CLS, MCR, PARAFAC, classification, instrument standardization, advanced preprocessing, hierarchical modeling, batch analysis, and many other multivariate analyses tools. Users can quickly manage data, and perform analyses for interpretation, model development, and deployment. Solo models can be exported for implementation in a variety of environments, and with the MIA_Toolbox add-on, Solo becomes a multivariate (hyperspectral) image analysis tool.
	PLS_Toolbox	A collection of essential and advanced chemometric routines	Tools work within the Matlab computational environment. It contains tools that chemical engineers, analytical chemists, other scientists, and data modelers require to explore their data and build predictive models.

interest in selling instruments without requiring the user to calibrate them.

The final type in “software” is not readily definable but consists of a group of miscellaneous offerings that provide something other than hardware (for example, nondigitized spectral libraries).

Advanced Chemistry Development (ACD/Labs) provides an informatics system that enables organizations to establish effective impurity control strategies based on assembled chromatographic, analytical, and chemical information, in a single environment.

BioRad is offering a 2018 version of its KnowItAll package that includes upgraded software and new and expanded databases.

Eigenvector Research has a stand-alone software package that implements its key algorithms without needing MATLAB support.

Fiveash Data Management provides spectral libraries for different classes of materials, including benzene, toluene, ethylene, and xylenes (BTEX), dyes, and essential oils using various types of spectroscopy, including attenuated total reflectance (ATR), vapor-phase FT-IR, and Raman spectroscopy. The BTEX Mixtures models two- to six-component mixtures of benzene, toluene, ethylbenzene, *o*-xylene, *m*-xylene, and *p*-xylene.

Horiba Scientific's new software package includes three key programs: NavMap, NavSharp, and ViewSharp.

Spectral Evolution's software package is now available with the GeoSPEC High Resolution Library EZ-ID mineral identification software.



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Table XI: Software products (continued)			
Company Name	Product Name	Product Type	Applications and Unique Features
Eigenvector Research, Inc.	MIA_Toolbox	Advanced hyperspectral image analysis	MIA_Toolbox software expands the already comprehensive functionality found in PLS_Toolbox and Solo with image-specific and image-enabled function to make analysis of multivariate images simple and intuitive.
	Solo_Predictor	Stand-alone prediction engine for use with PLS_Toolbox and Solo models	Solo_Predictor software is designed to be an easy, flexible, and economical way to use PLS_Toolbox and Solo models online to transform measured data to useable information. It includes a wide range of interfacing options to simplify connection to existing clients and data management systems. It supports all preprocessing methods available in the custom preprocessing interface of PLS_Toolbox and Solo, all standard PLS_Toolbox and Solo model types, and instrument standardization developed in PLS_Toolbox or Solo in the new CalTransfer GUI. Version 3.9
	Model_Exporter	Exporter for PLS_Toolbox and Solo models	Model_Exporter software exports PLS_Toolbox and Solo models to a stand-alone "predictor" script that provides a simple-to-implement recipe to perform model predictions. The result is low overhead, fast predictions for third-party software packages without the need for outside libraries or toolboxes. The software provides a fast, flexible path to deploying models for embedded, handheld, and portable devices. Applications: Predictions for handheld or embedded-computation devices, and high-throughput applications requiring high-speed data manipulation and calculations. On-line predictions can be made using Matlab Labview or Symbion software.
Fiveash Data Management, Inc.	FDM ATR BTEX Mixtures	Spectral library	The FDM ATR BTEX Mixtures spectral library models two- to six-component mixtures of benzene, toluene, ethylbenzene, <i>o</i> -xylene, <i>m</i> -xylene, and <i>p</i> -xylene. Users can search the full library and refine results by reducing the number of components. Users can generate reports or export graphics with the FDM SearchFaster software. Results from running and searching ATR-FT-IR spectra can be obtained in 1–2 min.
	FDM HiRes VPFTIR BTEX Mixtures	Spectral library	Same as the above except using FT-IR spectroscopy.
	FDM Raman BTEX Mixtures	Spectral library	Same as the above except except using Raman spectroscopy.
	FDM Raman Dyes	Spectral library	This new Raman spectral library covers dyes and pigments used in many sectors. The spectra cover 200–3400 cm^{-1} and were run on a Thermo DXR SmartRaman system using autoexposure and white light intensity correction. When needed, baseline correction was done manually. Matching FT-IR spectra are found in the FDM ATR Dyes library.
	FDM Raman Essential Oils	Spectral library	This new Raman spectral library covers essential oils and food oils used in the flavor and fragrance, food, and cosmetics industries. The spectra cover 200–3400 cm^{-1} and were run on a Thermo DXR SmartRaman system using autoexposure and white light intensity correction. When needed, baseline correction was done manually. Matching FT-IR spectra are found in the FDM ATR Essential Oils library.
Horiba Scientific	EasyNav	Raman imaging software package	The EasyNav software package features three modules. The NavMap module shows the global sample and the zoomed region of interest within the sample. The NavSharp module delivers real-time navigation on a sample image with any topography. The ViewSharp module constructs an image in which all surfaces are in focus simultaneously, and creates a 3D topography image.
Spectral Evolution	GeoSpec	High-resolution mineral library for EZ-ID	EZ-ID mineral identification software is now available with the GeoSpec high resolution library. The library includes known samples from the Colorado School of Mines Museum collection. There are more than 237 individual minerals and over 600 scans with multiple scans of different minerals. The GeoSpec library is a new add-on mineral spectral library for EZ-ID software with high-resolution scans. With the availability of the GeoSpec high resolution library, EZ-ID software users have access to three libraries (in addition to GeoSpec, the USGS and SpecMin libraries are available) for a total of 2700 spectra for 1047 minerals.

Table XI: Software products (continued)

Company Name	Product Name	Product Type	Applications and Unique Features
Spectro Analytical Instruments, Inc.	Spectro ICP Analyzer Pro	Software package	This new software delivers an improved and more-intuitive experience plus ease and speed for rapid retrieval and processing of results with total traceability. Recalculations, even of large amounts of data, are up to 1500 times faster. Modules and plug-ins are user-customizable. Software management system determines user rights, provides complete traceability, and delivers solid security. Traceability function stores all versions of a result. All changes, including user identification and timestamps, are logged as clear text for audit-trail use.
Wasatch Photonics	Enlighten	Spectroscopy operating software	This new spectroscopy software allows spectrometer users to quickly and easily collect Raman, absorbance, transmission, reflection, or scope mode spectra. Features include the ability to view spectra live, overlay current data with previous scans, perform instant peak finding, or export spectral data for further analysis as single or continuous-running scans. Software development kits are also freely available to enable development of software for specific platforms.
Wiley	Mass Spectra of Designer Drugs 2018	Spectral database	This spectral database features 26,459 mass spectra and 20,381 unique compounds predominantly classified as novel psychoactive substances (NPS). There are over 30 subcategories of compounds present such as amphetamines, cannabinoids, and benzodiazepines. The mass spectra found in this mass spectral reference library were compiled by Editor Peter Rösner and were extensively reviewed by the mass spectral experts Giselher Fritschi and Thomas Junge.

Spectro Analytical Instruments has a new software package that delivers a greatly improved and more intuitive experience plus unequaled ease and speed for the rapid retrieval and processing of results with total traceability and natural, streamlined workflows backed by ultrafast data processing.

Wasatch offers spectroscopy software that allows spectrometer users to quickly and easily collect Raman, absorbance, transmission, reflection, or scope-mode spectra at no additional cost. Features include the ability to view spectra live, overlay current data with previous scans, perform instant peak finding, or export spectral data for further analysis as single or continuous-running scans. The company also offers a software development kit.

Wiley is providing a mass spectral library of designer drugs, the Sigma-Aldrich library of Raman spectra, and the NIST 2017 library of mass spectra.

Accessories

The large number of accessories introduced this year (Table XII) covers the two main features needed: preparation of a sample for analysis or new ways to bring the sample into position for analysis. In all cases, the idea is to remove a pain point either to simplify the laboratory workflow or to ensure a sample is brought into position efficiently.

High-throughput analysis got attention with both ATR and terahertz Raman new products. Past years have seen developments around fluorescence, so these devices are bringing new flexibility to screening laboratories.

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Table XI: Software products (continued)			
Company Name	Product Name	Product Type	Applications and Unique Features
Wiley	Sigma-Aldrich	Library of Raman spectra	Wiley, on behalf of Merck KGaA Darmstadt, Germany, releases the Sigma-Aldrich Library of Raman Spectra, featuring over 6480 Raman spectra in the 4000–100 cm ⁻¹ range for over 6100 unique compounds with the Sigma-Aldrich catalog number for each record. The library can be accessed through the Wiley Spectra Lab IR, Raman, UV-vis, and NIR collection, which features over 345,000 spectra.
	NIST 2017 Mass Spectral Library	Library of mass spectra	The Wiley Registry/NIST mass spectral library is designed to increase instrument efficiency and staff productivity with replicate spectra and >3 million chemical names and synonyms to provide a high rate of correct identification and aid in classical EI, exact mass, and other methods of identification. The 11th edition EI library contains >1.6 million EI and MS/MS mass spectra collected by Dr. Fred McLafferty, the NIST Mass Spectrometry Data Center, and Wiley Science Solutions. The new release contains >1 million GC-MS spectra for >730,000 unique compounds. This library also features >650,000 LC-MS spectra for more than 15,000 unique compounds. This package contains the recently improved NIST MS Search software (2.3g), which includes improvements in search algorithms and the addition of hybrid searching to find spectra for compounds that differ by one inert group.

Table XII: Accessories				
Company Name	Product Name	Product Type	Measurement Mode	Applications and Unique Features
Advion	Open Port Sample Interface	Sample interface	Mass spectrometry	This sampling interface is designed for simple sampling of solids, liquids, and sample preparation tips and fibers. Paired with the electrospray ion source of the company's Expression compact mass spectrometer, the product incorporates an open port of continuous small-flowing volume of solvent directly into the mass spectrometer. Any soluble sample touching the port is analyzed by the mass spectrometer in seconds.
Anton Paar	Multiwave 7000	High pressure, high temperature digester	N/A	The Multiwave 7000 digester is designed for fast, automated sample digestion of any type of material. The system enables digestions at 300 bar and 200 °C of up to 24 different samples at a time. Automated pressurization and depressurization, an integrated cooling system, and a range of vial types including quartz, PTFE, and disposable glass vials are available. The system sends automated email notifications of completed runs and can be remotely controlled via VNC from a computer or mobile phone.
Czitek LLC	Microm ATR ₀	ATR accessory	ATR	The MicromATR ₀ ATR accessory includes fixed optics, a continuous force press, and digital readout to ensure reproducible results on solid materials. The compact ATR accessory is designed for use in most commercially available FT-IR instruments. New: Variable load technology enables operators to incrementally adjust the pressure to the desired setpoint using the coupled force readout. This combination eliminates small pressure-induced differences seen in standard ATR presses, simplifying the quantification of solids by ATR. By combining the new press technology with quantification software tools, quantification of solid samples with ATR is achievable.
High-Purity Standards	100 µg Alpha Quartz on PVC Filters	Certified reference material	N/A	This industrial hygiene-air monitoring certified reference material mimics the workplace sampling of α-quartz silica on 37-mm PVC filters. This kit includes five spiked filters and two blanks. The kit can be used for method development or quality control in the analysis of silica collected on PVC filters, or for practice in preparation for proficiency tests. The kit comes with an ISO Guide 34 certificate of analysis is traceable to NIST SRMs 2955 and 3150. This product is patterned after proficiency test items. It allows analysts to work with a known concentration before analyzing an unknown.
JEOL USA	Royal HFX	NMR probe	NMR	The probe's magnetic coupled probe technology offers a high degree of flexibility and sensitivity. The dual-tune mode allows for a wide variety of advanced NMR experiments including ¹ H{ ¹⁹ F}, ¹⁹ F{ ¹ H}, ¹³ C{ ¹ H, ¹⁹ F}, and many unique ¹³ C{ ¹ H, ¹⁹ F} correlation experiments, providing the flexibility to simplify spectral assignments of modern complex fluorine-containing compounds. There is no compromise in ¹³ C or X performance in either single tune ¹ H or ¹⁹ F mode or ¹ H- ¹⁹ F dual-tune mode. The probe is the only NMR probe that uses magnetic coupling as an efficient "on/off" switch for the high frequency coil to be dual-tuned to ¹ H and ¹⁹ F or single tuned to each. There is no loss in RF or signal-to-noise ratio performance relative to the standard Royal Probe for ¹ H, ¹⁹ F, ¹³ C, or X experiments. The autotune compatibility allows easy switching between modes.

Table XII: Accessories (continued)				
Company Name	Product Name	Product Type	Measurement Mode	Applications and Unique Features
JM Science Inc.	UV Quartz Cells	UV quartz cells	UV-vis	Each cell is packaged in an individual plastic case with a PTFE lid. The UV quartz cells have a "U" shaped bottom.
Ondax, Inc.	Low-frequency Transmission Raman Probe Accessory	Raman probe accessory	Raman	The transmission Raman accessory for the Ondax low-frequency terahertz-Raman probe enables fast, easy transmission, low-frequency Raman measurements on tablets and vials. Compatible with the Ondax TR-Probe platform, the accessory provides the best method to get average measurements over an entire sample volume, minimizing the signals of coatings or other materials. With up to 10x stronger signals in the low frequency region, quantification of formulated mixture components is enhanced, improving analysis of molecular structure, such as polymorphs and crystalline or amorphous forms.
	TR-WPS	Automated high-throughput screening system	N/A	The new TR-WPS automated well-plate measurement system combines high-throughput screening capability with the company's low-frequency terahertz Raman technology to automatically capture the entire Raman spectrum from -800 cm^{-1} to $+2800\text{ cm}^{-1}$ for common well-plate measurements. Ideal for screening and identification of polymorphic compounds and cocrystals, or quantifying degree of crystallinity in pharmaceuticals. The system is designed to deliver fast, fully automated, sensitive, and reliable measurements of both chemical composition and molecular structure. It is compatible with all standard well-plates including custom sample substrates.
PIKE Technologies	AutoATR	ATR accessory	ATR	At the heart of the AutoATR accessory is an ATR crystal made from $500\text{-}\mu\text{m}$ thick silicon that has been functionalized with multiple microprisms, which couples the light into the crystal. The thin crystal profile offers a full mid-IR spectral range from 5000 to 400 cm^{-1} . There are 24 individual and removable crystals mounted in a 24-well plate.
	Jackfish	Spectroelectrochemical cell	ATR-SEIRAS	This spectroelectrochemical cell is designed for surface-sensitive spectroelectrochemistry with the ATR-SEIRAS technique. It is designed and tested for use with the PIKE Technologies VeeMAX III variable angle specular reflectance accessory. High-quality infrared spectra can be obtained from submonolayer amounts of material at the electrode-solution interface. By using the PIKE face-angled VeeMAX Si crystal, results can be obtained that outperform a conventional Si hemisphere in terms of signal-to-noise ratio.
Savillex Corporation	HPX Series	Inert hotplates	N/A	Design features incorporated into the HPX series inert hotplates provide temperature uniformity across the heating surface for greater control over sample digestion and evaporation. Incorporating more cartridge heaters than are typically used in inert hotplates reduces temperature variability across the heating surface. In addition, the use of ISO-molded, low-porosity graphite gives good thermal conductivity and also allows for a high integrity PFA coating that protects the heating block, prevents corrosion and contamination, and extends operating life.
Specac	Apex	Quick-release die	XRF	The Apex quick-release die is an intuitive substitute for awkward and time-consuming sample pellet extraction. The die makes routine pellet extraction simple and faster with the entire cycle taking as little as 2–3 min from loading the sample to retrieving the finished pellet. It can be used with the Specac Autotouch press for XRF applications.
Spectra Solutions, Inc	Fiber Optic Raman Probes	Raman probes	Raman scattering	These probes offer a very compact form factor, user-replaceable fiber optic cables, and user-replaceable focusing lens barrel including a high-pressure (6000 psi) and high temperature ($300\text{ }^{\circ}\text{C}$) version. A fully sealed and purgeable probe housing version is available. Probes are available for various lasers including 785-, 670/671-, 633-, and 532-nm wavelengths.
ST Japan USA LLC	EZ-Slicer	Sample preparation	N/A	The new EZ-Slicer compact precision cutting device enables users to easily and accurately cut sections of thin materials such as packaging materials, films, laminates, paper, and fibers. Perfect control of section thickness can be achieved down to $20\text{--}30\text{ }\mu\text{m}$ and even sections of several micrometers thickness can be cut. The cutting angle can be set individually at any angle between 45° and 90° . The sample can be horizontally rotated to up to 10° .
Thermo Fisher Scientific	ConservatIR	FT-IR external reflection accessory	FT-IR	This articulated optomechanical arm measures samples too large to fit into an FT-IR spectrometer sample compartment. The articulated arm simplifies sample analysis with the object in front of, below, or above the spectrometer sample compartment. Comes standard with a specular-diffuse sampling head with a diamond ATR sampling head as an option. Ideal for art conservation studies.

Table XIII: Components				
Company Name	Product Name	Product Type	Measurement Mode	Applications and Unique Features
Cobolt AB	08-01 Series lasers	Lasers	N/A	The 08-01 series lasers consist of high performance, ultracompact, single longitudinal mode (SLM) diode pumped lasers (08-DPL) up to 400 mW and narrow linewidth diode lasers (08-NLD) up to 500 mW, all having high wavelength stability and spectral purity. With integrated electronics and an integrated optional optical isolator and clean up filter, the lasers are easily integrated into high-end Raman-based systems or other analytical instrumentation. New wavelengths are 457, 473, 515, 660, and 1064 nm.
Electro-Optics Technology, Inc.	Tornos Series	Compact optical isolators	N/A	These isolators eliminate frequency instability in single-frequency laser diodes and parasitic oscillations resulting from amplified spontaneous emission (ASE) in amplified laser systems, and generally protects a laser system from underperforming or damage from optical feedback. The isolators feature a small footprint, high transmission, and are designed to be integrated into small, compact laser systems. The Tornos Series compact optical isolators feature a smaller package in both diameter and length, a higher transmission of >33 dB, and an increased isolation of >95%, and they are tailored to OEM applications. Applications: Raman spectroscopy, DNA sequencing, remote sensing.
Energetiq Technology	EQ-9	Laser-driven light source	N/A	The EQ-9 LDLS laser-driven light source offers the highest radiance and irradiance available in a broadband white light source. The light source features a compact lamp house, with clean construction that ensures long life and ultimate stability. With a 170–2100 nm wavelength range, and a choice of dual-beam output or a single-beam output with retroreflector, the light source is flexible for a broad variety of applications.
Laser Components USA, Inc.	PB50/55 and PB27/30	Lead salt detectors	N/A	In the PB50/55 and PB27/30 lead salt detectors, thermoelectric coolers (TEC) for PbSe/PbS detectors leverage mid-IR detection. Cooling PbSe/PbS detectors increases sensitivity and extends the peak wavelength response. These improved heat pumps achieve the same ΔT with less required cooler power. Better feedback control of the TEC top stage maintains detector temperature stability. Combined with proper heat sink design and identifying the optimum operating temperature, these TECs help to provide the best possible detection in the mid-IR.
Princeton Instruments	Blaze	CCD camera for spectroscopy	NIR	The HR sensors in the Blaze CCD camera deliver the highest QE in the NIR region, with ~90% from 690 to 960 nm, ~95% from 800 to 900 nm, and 75% QE at 1000 nm, which is 2–4 times higher than conventional CCD cameras. With the LD sensor option, the camera minimizes dark current, ideal for long exposures. Exclusive SeNsR technology allows rapid on-chip shifting and accumulation of sample and reference data. It can be cooled to true -100 °C with 20 °C liquid assist without condensation.
Spectrolight Inc.	Flexible Wavelength Selector	Wavelength selector	N/A	The Flexible Wavelength Selector (FWS) light filtering device combines the precision wavelength tuning and adjustable bandwidth of a monochromator with the uniform circular imaging aperture of a bandpass filter. Based on TwinFilm technology, the FWS is the a simple optomechanical device that precisely filters incoming light without losing or scrambling the spatial (image) information. It thus enables direct spectral imaging. Manual and fully automated (USB) tuning options are available.
	The Mighty Light Plus	White light source	N/A	The Mighty Light Plus (ML+) high power white light source (350–2500 nm) delivers 10 times higher spatial brightness than any other available product. Specifically, the light source outputs up to 7 W from a 10-mm diameter, detachable, armored light guide. This output provides high spatial uniformity suitable for both wide-field and focused spot illumination applications. Plug-and-play accessories include an optional collimator for use in free space optics applications.
Spectrum Scientific, Inc.	Freeform Mirrors	Mirrors	N/A	Freeform mirrors are curved mirrors with no axial symmetry that allow compound compensation, meaning that a single optic can replace multiple optics, reducing the system volume and allowing for increased aberration correction. This design makes them suitable for any application where space is at a premium and a compact design is essential or improved performance is required. Examples of applications include space and defense systems, telecommunications, and analytical or spectroscopic instrumentation. Previously, the cost and complexity of manufacturing free-form mirrors meant that it wasn't until recently that they have entered main stream usage with the use of the replication process, meaning that today's freeform optic is a high volume, high fidelity, high performance optic that in most cases is diffraction limited.

Advion provides an open port sampling interface (OPSI) that is designed for simple sampling of solids, liquids, and sample preparation tips and fibers. The interface is designed to pair with the

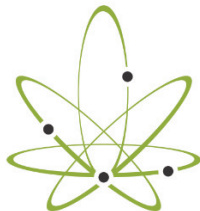
electrospray ion source of the company's Expression compact mass spectrometer.

Anton-Paar's Multiwave 7000 system enables fast, automated sample digestion of any type of material by digesting

at the high temperature and pressure of 300 bar and 200 °C for up to 24 different samples at a time.

Czitek shows the MicromATRQ ATR accessory with digital force readout. The

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accessory includes fixed optics, a continuous force press, and digital readout to ensure reproducible results on solid materials. The compact ATR accessory can be used with most commercially available FT-IR spectrometers.

High Purity Standards offers a certified reference material that mimics the workplace sampling of α -quartz silica on 37-mm polyvinyl chloride (PVC) filters. This kit includes five spiked filters and two blanks.

JEOL's patented magnetic coupled probe technology offers significantly more flexibility and sensitivity than alternatives.

JM Science provides a large selection of high-quality UV quartz cells.

Ondax has a transmission Raman probe accessory designed to enable fast, easy, low-frequency transmission Raman measurements on tablets and vials.

PIKE Technologies has the AutoATR accessory, which comprises a new ATR crystal that has been functionalized with multiple micropisms.

Savillex provides hotplates that give unmatched temperature uniformity across the heating surface, providing greater control over sample digestion and evaporation.

Specac Limited provides a quick-release die that is an intuitive solution to awkward and time-consuming sample pellet extraction.

Spectral Solutions provides very compact form factor, user-replaceable fiber-optic cables, and a user-replaceable focusing lens barrel, including a high-pressure (6000 psi) and high-temperature (300 °C) version

The EZSlicer compact precision cutting device from S.T. Japan-Europe GmbH is designed to easily and accurately cut sections of thin materials such as packaging materials, films, laminates, paper, and fibers. It allows control of section thickness down to 20–30 μm .

Thermo Fisher Scientific provides an articulated opto-mechanical arm that measures samples too large to fit into an FT-IR spectrometer sample compartment. The articulated arm simplifies sample analysis with the object in front, below, or above the spectrometer sample compartment.

Components

When it comes to components (Table XIII), we raise the same question every year: What's the difference between a component and an accessory? We say this so that we don't get in arguments over the classification of some particular instrument or other. So, it still needs to be repeated: A component is something that can be used in the construction of an instrument and becomes an inherent part of it; if it's not there, then the instrument will not work or at least be severely degraded. An accessory is a device that can be used optionally in conjunction with an instrument and is generally external to it. The instrument will work just fine without the accessory, but it extends the instrument's capabilities (for example, a liquid flow cell for an instrument innately designed to measure solid samples). The accessory can be removed to return the instrument to its previous performance level, whereas a component generally cannot be removed except by a factory trained expert.

This year, optical components seemed to predominate. An interesting development in components involved the release by two companies, Spectro-Light and Energetiq Technology, of new white light sources of high luminosity and performance. In a field dominated recently by lasers, this is a striking development. Most laser system manufacturers were discussing upgrades and updates. There was also discussion of new mirror processing and a novel approach to wavelength selection.

Cobolt has released several new wavelengths in its 08-01 series of lasers, which consists of high performance, ultracompact, single longitudinal mode (SLM) diode pumped lasers (08-DPL) up to 400 mW. Available wavelengths include 457, 473, 515, 660, and 1064 nm.

Electro-Optics Technology's compact optical isolators eliminate frequency instability in single-frequency laser diodes, parasitic oscillations resulting from amplified spontaneous emission (ASE) in amplified laser systems, and generally protect your laser system from under-performing or damage resulting from optical feedback.

Energetiq Technology provides the EQ-9 LDLS laser-driven light source, which offers the highest radiance and irradiance available in a truly broadband white light source.

Laser Components makes superior thermoelectric coolers (TEC) for PbSe/PbS detectors leverages mid-IR detection. These improved heat pumps achieve the same ΔT with less required cooler power. Better feedback control of the TEC top stage maintains detector temperature stability.

Princeton Instruments has a CCD camera for spectroscopy. The company's Blaze proprietary HR sensors deliver the highest quantum efficiency (QE) in the NIR region, with ~90% from 690 to 960 nm, ~95% from 800 to 900 nm, and 75% at 1000 nm.

Spectrolight provides optical accessories, including a bright white light source and a wavelength selector that can provide interference-filter optical characteristics.

Spectrum Scientific provides Freeform mirrors, which are curved mirrors with no axial symmetry that allow compound compensation, meaning that a single optic can replace multiple optics, thereby reducing the system volume and allowing for increased aberration correction.

Reference

- (1) <https://pittcon.org/exhibitor/pittcon-demographics/>.

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 *Spectroscopy's* Editorial Advisory Board and is a Senior Manager, Product Applications at Thermo Fisher Scientific in Madison, Wisconsin. Direct correspondence to hmark@nearinfrared.com ■

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

McPHERSON

Wavelength Dependent Performance Loss in the Ultraviolet

Lori Krupa, Dave Riley, and Erik Schoeffel, McPherson

Optical samples measured in a vacuum change while we watch—the vacuum environment contributes to measurable changes in optical performance. We measured optical transmission samples in high vacuum and then in dry nitrogen. We then quantified vacuum environment contamination and polymerization in a manner easily demonstrated and repeated. These results are useful for metrology laboratories and manufacturers of analytical instruments, semiconductor process control, material scientists, and other researchers. It may be time to revisit standards for the deep ultraviolet 120 to 300 nm region!

We measured a series of samples in a vacuum spectrophotometer (1). It uses a high vacuum turbomolecular pump with a molecular drag roughing pump. Vacuum level during measurements was better than 5×10^{-5} Torr. The instrument used a 30-Watt deuterium lamp with magnesium fluoride window, a scanning monochromator, and collimated measuring beam. All sample measurements have a new reference and correction scan. All samples were tested from 115 to 220 nm. The samples are magnesium fluoride windows 25×2 mm thick. Magnesium fluoride was used because it transmits ultraviolet light well, especially less than 140 nm. Samples were handled with gloves and exposed to the lab atmosphere as little as possible. Orientation marks maintained consistent mounting. Cleaning consisted of methanol and Kimwipe™ to remove particulate or gross contamination and UV-ozone scrubbing.

We then measured the same samples in a nitrogen purged spectrophotometer. This was the same spectrophotometer that was used for vacuum testing except the vacuum pump was removed and dry nitrogen gas flowed instead. Each sample was cleaned before and the transmission was measured.

The experiment shows that regardless of how clean a sample is, or how good the vacuum level, some wavelength dependent losses occur in the vacuum environment. Wavelength dependent

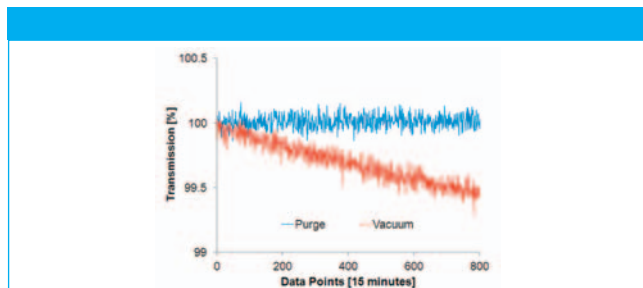


Figure 1: Deep ultraviolet transmission loss at 121 nm occurs rapidly in vacuum systems (red) and is much more stable in nitrogen purge (blue).

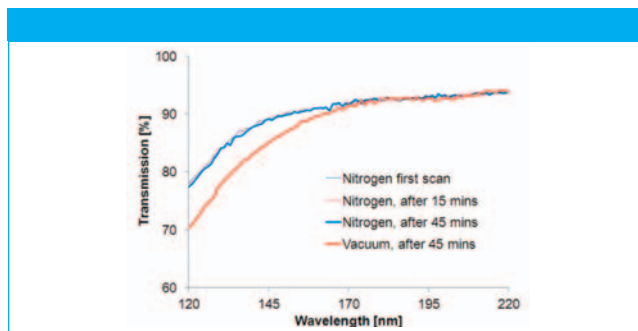


Figure 2: Wavelength dependent performance loss of plasma cleaned sample in vacuum (red) compared to same (cleaned) sample measured in nitrogen purge (blue) at 15, 30, and 45 min.

transmission loss is most obvious at shorter wavelengths and on clean samples. These types of materials are transmitting or reflecting wavelengths very easily absorbed by various contaminants (2). The experiment also shows that the cleaner a surface is, the quicker contamination begins to be measureable. All measured values are better or higher in nitrogen. Even with no UV illumination, nucleation or particle and ion condensates (3) in vacuum result in optical performance losses. Nitrogen system performance remains stable over longer timescales too.

Improved and reliable cleaning methods have allowed us to serially clean a sample and subsequently measure it in different ways. The measurement and quantification of vacuum environment contamination on UV transparent materials becomes obvious when compared to measurements made in purged systems. Measurements in other purged systems indicate the vacuum environment is the cause of contamination that may become polymerized, and UV exposure alone does not polymerize contamination until the vacuum helps deposit it. Implementing reproducible cleaning methods, in combination with a nitrogen purged VUVAS spectrophotometer provides the most accurate deep ultraviolet data currently possible.

References

- (1) McPherson specification sheet VUVAS 2000.
- (2) J. R. Vig, UV/Ozone cleaning of surfaces, *Surface Contamination*, (1979).
- (3) D.M. Mattox, "Handbook of Physical Vapor Deposition (PVD) Processing," 142, Elsevier (2010).

McPherson

7-A Stuart Road, Chelmsford, MA 01824
tel. (978) 256-4512, fax (978) 250-8625
Website: www.mcphersoninc.com

PRODUCTS & RESOURCES

Atomic emission spectrometer

LECO's GDS9000 glow discharge atomic emission spectrometer is designed for routine bulk elemental determination in most conductive solid metal matrices. According to the company, the spectrometer is suitable for analysis of steel, iron (including as-cast), aluminum, copper, zinc, nickel, cobalt, tungsten, and titanium.

LECO Corporation, St. Joseph, MI; www.leco.com



Sample preparation primer

A primer titled "Microwave-Assisted Pharmaceutical/Nutraceutical Sample Prep for USP <232>/<233>/<2232>" is available from Milestone. According to the company, the primer provides a better understanding of sample preparation for ICP and ICP-MS techniques used in pharmaceutical and nutraceutical laboratories, and provides guidance on sample preparation technology.

Milestone, Inc., Shelton, CT; www.milestonesci.com/usp-232-233-compliance



Raman polymer analysis application note

An application note from Renishaw describes how Raman imaging provides the power and flexibility to investigate all polymer types to provide chemical information and high-resolution 2D and 3D chemical images. According to the company, applications range from investigation of polymer crystallinity, and understanding coating layers, to identification of microplastic contamination in the environment.

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



Polymer fluorescent references

Starna's second-generation polymer fluorescent references are designed for wavelength calibration and the monitoring of instrument performance in fluorescent applications. According to the company, the new references are based on new proprietary dyes and provide increased stability and resistance to photobleaching, allowing for their use as relative photometric intensity references.

Starna Cells, Inc., Atascadero, CA; www.starnacells.com



Raman opioid analysis application note

An application note titled "FT-Raman: An Invaluable Addition to the Forensic Arsenal to Combat the Opioid Epidemic" is available from Thermo Fisher Scientific. The application note reportedly describes the advantages of using Fourier transform Raman spectroscopy to detect and identify fentanyl and other illicit drugs.

Thermo Fisher Scientific, Madison, WI; www.thermofisher.com/spectroscopy

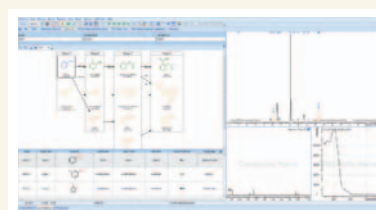


Informatics system

ACD/Labs' LUMINATA informatics system is designed to enable organizations to establish effective impurity control strategies based on assembled analytical and chemical information, in a single environment.

According to the company, the system provides data aggregation and visualization for substance impurity characterization.

ACD/Labs, Toronto, Ontario, Canada; www.acdlabs.com



NIR sensor

The NIRONE near-infrared (NIR) sensor from Spectral Engines is designed with a Fabry-Perot microelectromechanical systems (MEMS) sensor and light sources. According to the company, a typical signal-to-noise ratio is >10,000 for a single measurement.

Flash Photonics, a distributor for Spectral Engines, Redmond, WA; www.flash-photonics.com



UV-vis spectrometer

The Ocean HDX UV-vis spectrometer is designed as an optical bench with components that provide high throughput, low stray light, and thermal stability for integrated, industrial, and research applications. According to the company, the spectrometer is responsive from 200 to 925 nm, with thermal stability of +/-1.0 pixels from 0 to 40 °C.

Ocean Optics, Largo, FL; hdx.oceanoptics.com

Erratum: The stated response range was previously misstated as 200 to 290 nm. The correct range is 200 to 925 nm.



Compact Raman laser

Ondax's Mini-Benchtop laser is designed for Raman spectroscopy. According to the company, the laser includes manual power controls, a touchscreen display, and an emergency stop, delivering better than 1% power stability and less than a 1-min warm-up. It is available in powers up to 500 mW at wavelengths from 405 nm to 1064 nm.

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



FT-NIR system

PerkinElmer's Spectrum Two N transportable FT-NIR system is designed for NIR analysis. According to the company, the system has plug-and-play accessories and is suitable for users with different levels of expertise, including novices and seasoned professionals.

PerkinElmer,
Waltham, MA;
www.perkinelmer.com



Spectroelectrochemical cell

The Jackfish SEC spectroelectrochemical cell from PIKE is designed for surface-sensitive spectroelectrochemistry with attenuated total reflection– surface-enhanced infrared absorption spectroscopy. According to the company, the three-electrode cell can be purged with inert gas to remove dissolved oxygen.

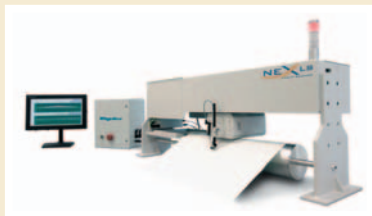
PIKE Technologies,
Madison, WI;
www.piketech.com



Scanning multielement XRF analyzer

The Rigaku NEX LS scanning multielement process coatings analyzer is designed with energy dispersive X-ray fluorescence technology. According to the company, the analyzer provides nondestructive analyses for elements ranging from aluminum through uranium.

Applied Rigaku Technologies,
Austin, TX;
www.rigakuEDXRF.com



Compact FT-IR spectrophotometer

Shimadzu Scientific's IRSpirit FT-IR spectrophotometer is designed for space efficiency in the laboratory, allowing access from two sides and providing a wide sample compartment. According to the company, the instrument includes a sealed interferometer that protects the beam splitter from both air and moisture.

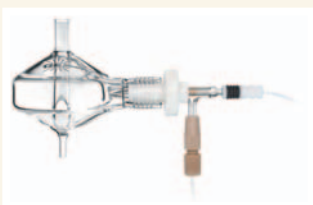
Shimadzu Scientific Instruments,
Columbia, MD;
www.ssi.shimadzu.com



Nebulizer

Glass Expansion's Helix CT (ConstantTorque) nebulizer interface reportedly is now available with all of the company's glass, PFA, and PTFE spray chambers. According to the company, the nebulizer's locking screw with built-in torque control mechanism provides a consistent seal of the PTFE ferrule against the nebulizer, making it impossible to overtighten or undertighten while ensuring a gas-tight seal.

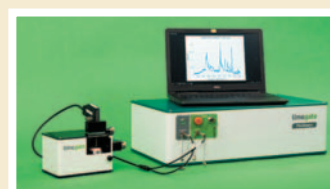
Glass Expansion, Inc., Pocasset, MA; www.geip.com/HelixCT



Raman spectrometer

The PicoRaman spectrometer from TimeGate is designed to minimize or eliminate background sample fluorescence using a combination of a picosecond laser and a picosecond detector. According to the company, the Raman scattering from the pulsed laser is prompt, and the fluorescence, which is delayed, is gated out by the detector.

Flash Photonics, a distributor for TimeGate Instruments, Ltd., Redmond, WA; www.flash-photonics.com



Spectrograph

Princeton Instruments' SpectraPro HRS-500 high-performance spectrograph is designed for multichannel fiber applications. According to the company, the option of two full 14 mm x 30 mm exit and two entrance ports allows for the mounting and operation of two detectors, or enables the instrument to operate as both a monochromator and a spectrograph.

Princeton Instruments, Trenton, NJ; www.princetoninstruments.com



NIR scanner

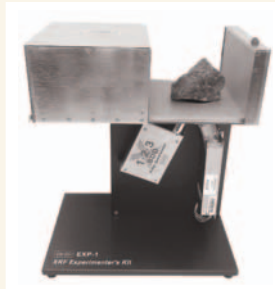
The NIRONE scanner from Spectral Engines is designed to pair wireless and Bluetooth connectivity with the company's NIRONE NIR sensor and light sources. According to the company, the battery-powered scanner is ready for measurements out of the box, and includes cloud-based analytics and a free demonstration and feasibility testing service. **Flash Photonics**, a distributor for Spectral Engines, Redmond, WA; www.flash-photonics.com



XRF kit

Amptek's XRF kit is designed to help users quickly begin doing elemental analysis via X-ray fluorescence. According to the company, the kit includes the company's X-123 complete spectrometer with a FAST SSD or SSD detector, a Mini-X USB Controlled X-ray tube, XRF-FP QA software, a sample enclosure, and test sample.

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



Microwave digestion system

CEM's MARS 6 sample preparation system now includes the contactless in situ iWave temperature sensor. According to the company, using light-emitting technology, the sensor renders the vessel transparent, enabling the determination of the temperature of the actual sample in real time. The sensor reportedly can measure the sample temperature of each vessel without the need for a control vessel, fiber-optic probes, or wires.

CEM Corporation, Matthews, NC; www.cem.com



Optical isolators

EOT's compact Tornos Series optical isolators are designed to provide high transmission in the forward direction while strongly attenuating light traveling in the reverse direction. According to the company, the isolators allow for isolation and transmission at a specific wavelength within the spectral bandwidth of the isolator.

Electro-Optics Technology, Inc., Traverse City, MI; www.eotech.com



FT-IR gas analyzer

The MBGAS-3000 FT-IR gas analyzer from ABB Measurement & Analytics is designed for multigas component analysis for combustion processes. According to the company, the analyzer is intended for continuous operation without the need for operator intervention and can be integrated into a continuous emission monitoring system.

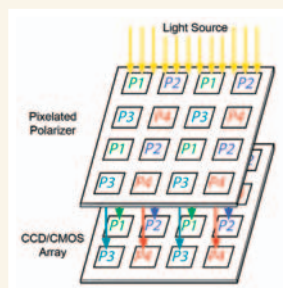
ABB Measurement & Analytics, Quebec, QC, Canada; www.abb.com/analytical



Polarizer arrays

Moxtek's pixelated polarizer arrays are designed to attach to charge-coupled device and complementary metal-oxide semiconductor cameras for real-time image and video acquisition. According to the company, standard pixel pitches range from 5.0 to 26.0 mm, and sizes ranging from 0.25 to 4 megapixel are used in the visible through long-wave infrared.

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



Spectrometer accessory

Edinburgh Instruments' Cryosphere accessory is designed for use with its FLS1000 spectrometer. According to the company, the accessory is used in measuring photoluminescence quantum yield from 77 K to 500 K, features a software-controlled cryostat inside an integrating sphere, and allows measurements of solids and powders.

Edinburgh Instruments, Livingston, UK; www.edinst.com



Calendar of Events

June

3–7 June 66th ASMS Conference on Mass Spectrometry and Allied Topics

San Diego, CA

www.asms.org/conferences/annual-conference/annual-conference-homepage

10–13 June Chirality 2018

Princeton, NJ

www.cvent.com/events/chirality-2018/event-summary-60224931d7c641328312754e3a7688e9.aspx

10–13 June 9th Nordic Conference on Plasma Spectrochemistry

Loen, Norway

nordicplasma.com

10–14 June XIII International GeoRaman Conference (GeoRaman 2018)

Catania, Italy

www.spectroscopyeurope.com/events/georaman-2018

10–15 June 13th International Conference on Synchrotron Radiation Instrumentation (SRI 2018)

Taipei, Taiwan

sri2018.nsrrc.org.tw/site/page.aspx?pid=901&sid=1157&lang=en

11–15 June ACHEMA 2018

Frankfurt am Main, Germany

www.achema.de/en/home.html

13–15 June 15th International HITRAN Conference (united with the 14th ASA conference)

Cambridge, MA

hitran.org/conferences/hitrان-15-2018

14 June Photonex Scotland, Photonics Exhibition and Conference

Scotland, UK

www.photonex.org/scotland/18/scotland-advances-in-photonics.html

17–20 June International Association for Spectral Imaging (IASIM) Conference 2018

Seattle, WA

www.spectroscopyeurope.com/events/international-association-spectral-imaging-iasim-conference-2018

17–22 June 24th International Conference on Spectral Line Shapes (ICSLS)

Glasnevin, Ireland

www.icsls2018.com/

19–22 June XVIII International Symposium on Luminescence Spectrometry: Fundamentals and Applications (ISLS 2018)

Brest, France

isls2018.sciencesconf.org

24–29 June European Conference on X-ray Spectrometry

Ljubljana, Slovenia

exrs2018.ijs.si

25–26 June 2018 RamanFest 2018: 6th International Conference on Advanced Applied Raman Spectroscopy

Tokyo, Japan

www.ramanfest.org

July

1–5 July European Magnetic Resonance Meeting (EUROMAR) 2018

Nantes, France

www.euromar2018.org/EventPortal/Information/EUROMAR18/HOME.aspx

15–19 July 15th International Conference on Surface X-ray and Neutron Scattering (SXNS15)

Pohang, Korea

www.sxns15.org

15–20 July Gordon Research Conference on In Vivo Magnetic Resonance: Challenging Assumptions About Magnetic Resonance Technology and Applications in a Changing World

Andover, NH

www.grc.org/in-vivo-magnetic-resonance-conference/2018

22–27 July 59th Annual Rocky Mountain Conference on Magnetic Resonance

Snowbird, UT

www.rockychem.com

29 July–2 August International Diffuse Reflectance Conference (IDRC 2018)

Chambersburg, PA

cnirs.clubexpress.com/content.aspx?page_id=22&club_id=409746&module_id=276194

August

1–2 August 3rd International Seminar on Photonics, Optics, and its Applications (ISPhOA 2018)

Surabaya, Indonesia

www.isphoa2018.org

October

15–16 October Laser Optics 2018

Paris, France

lasers-optics-photonics.pulsusconference.com

Short Courses

June

2–3 June Bioinformatics for Protein Identification

San Diego, CA

www.asms.org/docs/default-source/conference-short-course-descriptions/01-bioinformatics-for-program-identification.pdf?sfvrsn=2

4–6 June Mass Spectral Interpretation

Pittsburgh, PA

pacslabs.com/course/10massspectralinterpretationcourse.php

6–8 June Advanced Mass Spectral Interpretation

Pittsburgh, PA

pacslabs.com/course/20advancedmassspectralinterpretationcourse.php

14 June Spectroscopy Simplified - A Short Course on Infrared and Raman Spectroscopy

Paisley, UK

www.rsc.org/events/detail/31561/spectroscopy-simplified-a-short-course-on-infrared-and-raman-spectroscopy

July

16–20 July Infrared Spectroscopy I: Interpretation of Infrared and Raman Spectra

Brunswick, ME

www.ircourses.org

29 July Fundamentals of NIR

Chambersburg, PA

cnirs.clubexpress.com/content.aspx?page_id=22&club_id=409746&module_id=276201

29 July Basic Chemometrics

Chambersburg, PA

cnirs.clubexpress.com/content.aspx-

?page_id=22&club_id=409746&module_id=276201

29 July PAT

Chambersburg, PA

cnirs.clubexpress.com/content.aspx?page_id=22&club_id=409746&module_id=276201

29 July Networking

Chambersburg, PA

cnirs.clubexpress.com/content.aspx?page_id=22&club_id=409746&module_id=276201

August

25–26 August Fundamentals of Mass Spectrometry

Florence, Italy

www.imsc2018.it/courses.php

25–26 August Foodomics & Mass Spectrometry

Florence, Italy

www.imsc2018.it/courses.php

25–26 August Mass Spectrometry Imaging

Florence, Italy

www.imsc2018.it/courses.php

25–26 August Expanded Newborn Screening by Tandem Mass Spectrometry

Florence, Italy

www.imsc2018.it/courses.php

25–26 August Solid-Phase Microextraction: Comprehensive Overview of the Technology and Applications to Analytical Mass Spectrometry

Florence, Italy

www.imsc2018.it/courses.php

October

21–26 October Laser Induced Plasma Emission: From Atomic to Molecular Spectra

Atlanta, GA

www.scixconference.org/short-courses/workshop-list

21–26 October Advance Applications of LAICPOES, LAICPMS and LIBS

Atlanta, GA

www.scixconference.org/short-courses/workshop-list

21–26 October Intro to Raman with Imaging Applications

Atlanta, GA

www.scixconference.org/short-courses/workshop-list

21–26 October Basic Chemometrics

Atlanta, GA

www.scixconference.org/short-courses/workshop-list

21–26 October Classification of Unknown Materials Using Microscopy and Spectroscopy

Atlanta, GA

www.scixconference.org/short-courses/workshop-list

21–26 October Non-Linear Methods for Regression and Classification

Atlanta, GA

www.scixconference.org/short-courses/workshop-list

21–26 October Basics of Multivariate Modeling of Spectroscopic Data

Atlanta, GA

www.scixconference.org/short-courses/workshop-list

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References. Number the literature citations in the text consecutively in order of appearance and indicate them by Arabic numerals in parentheses. Number each reference separately. Group the references at the end of the manuscript in the order of their appearance in the text, not alphabetically.

Use Chemical Abstracts Service Source Index for journal abbrevia-

tions. Use the following format for references:

- (1) R. Salzer and H.W. Siesler, *Infrared and Raman Spectroscopic Imaging* (Wiley-VCH, Weinheim, 2009), pp. 90–103.
- (2) P. Matousek, *Appl. Spectrosc.* **60**, 1341 (2006).

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Lasers and Optics Interface Column

We also accept contributed manuscripts for the "Laser and Optics Interface" column. Tutorials, reviews, and experimental articles can all be suitable for this column.

Special Supplements

A number of supplemental issues are planned for 2018, for which we also invite contributions. Manuscripts for the supplements on IR, ICP & ICP-MS, portable/handheld spectroscopy, and food and beverage analysis should be 2500–3000 words long, plus up to eight figures and tables, and should include an abstract of approximately 150–200 words. We are still accepting submissions for the following issues:

ICP & ICP-MS supplement, September 2018

Submission deadlines:
Abstracts: June 11, 2018
Manuscripts: August 1, 2018

Food & Beverage Analysis supplement, October 2018

Submission deadlines:
Abstracts: June 8, 2018
Manuscripts: August 15, 2018

Portable/Handheld Spectroscopy supplement, November 2018

Submission deadlines:
Abstracts: June 7, 2018
Manuscripts: August 6, 2018

Current Trends in Mass Spectrometry supplement series

Our supplement series on mass spectrometry appears four times a year: in March, May, July, and October. Manuscripts for this series should be approximately 3500–4500 words long, including an abstract of approximately 150–200 words, plus up to eight figures and tables. We are still accepting submissions for the following issues:

Submission Deadlines:

October 2018 issue
Abstracts: May 8, 2018
Manuscripts: July 13, 2018

March 2019 issue
Abstracts: September 28, 2018
Manuscripts: December 1, 2018

May 2019 issue
Abstracts: November 5, 2018
Manuscripts: February 8, 2019

Contact Us

For more information about contributing to *Spectroscopy*, please contact

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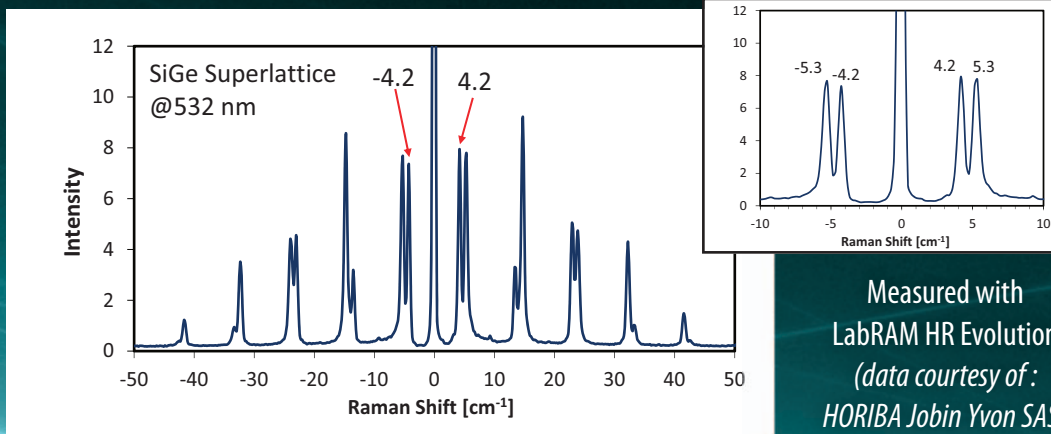
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Ad Index

ADVERTISER	PG#	ADVERTISER	PG#
ACD/Labs	21	Ocean Optics, Inc.	CV2
Amptek	5	Ondax, Inc.	25
Anton Paar US	9	OptiGate Corporation	CV3
CEM Corporation	15	PerkinElmer Corporation	CV4
Electro-Optics Technology	43	PIKE Technologies	29
Flash Photonics, Inc.	37	Princeton Instruments	13
Glass Expansion	30, 31	Renishaw, Inc.	33
Harrick Scientific Corporation	17	Rigaku GMG	8
jCanna, Inc.	49	Shimadzu Scientific Instruments	7
Magritek	41	Specac	27
McPherson	51	Sterna Cells, Inc.	39, 45
Milestone	CV Tip	StellarNet, Inc.	35
Moxtek, Inc.	11	Thermo Fisher Scientific	3
New Era Enterprises, Inc.	58		

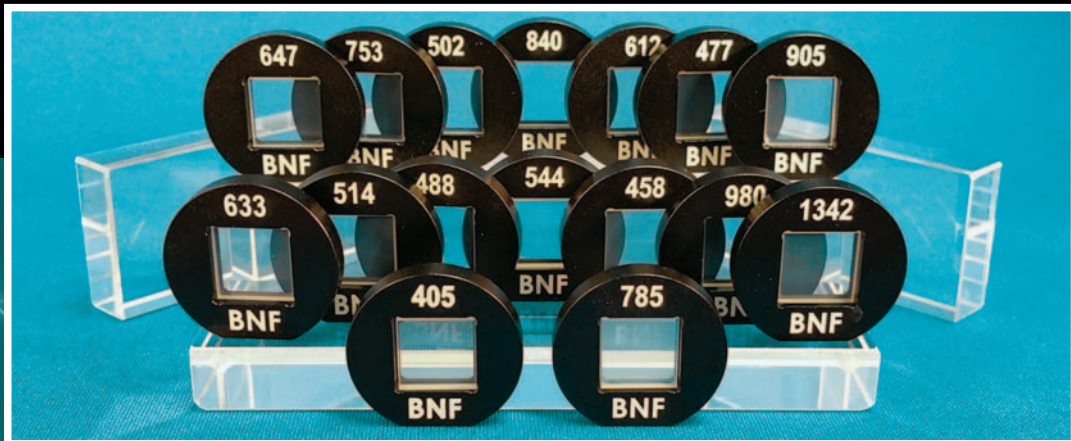
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568, 588, 594, 632, 660,
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HIGH-PERFORMANCE FT-NIR THAT GOES WHERE YOU GO

This transportable system is big on performance for all types of QA/QC samples

From pharmaceuticals to food, polymers to petroleum, the Spectrum Two N™ system delivers the highest levels of performance, sensitivity, and resolution, whether for simple QA/QC or advanced chemometric analyses – all on one flexible, portable system. Three new features – a plug-and-play Near Infrared Reflectance Module, a Heatable Transmission Module with multiple vial sizes, and a Remote Sampling Module with a triggered solids probe for through-container sampling – make it the most versatile small FT-NIR ever. Plus, simple, powerful software with 21 CFR Part 11 compliance modules provides additional peace of mind. The Spectrum Two N: It goes wherever your samples lead you.

Learn more at www.perkinelmer.com/SpectrumTwoN



Spectrum Two N™ FT-NIR Spectrometer