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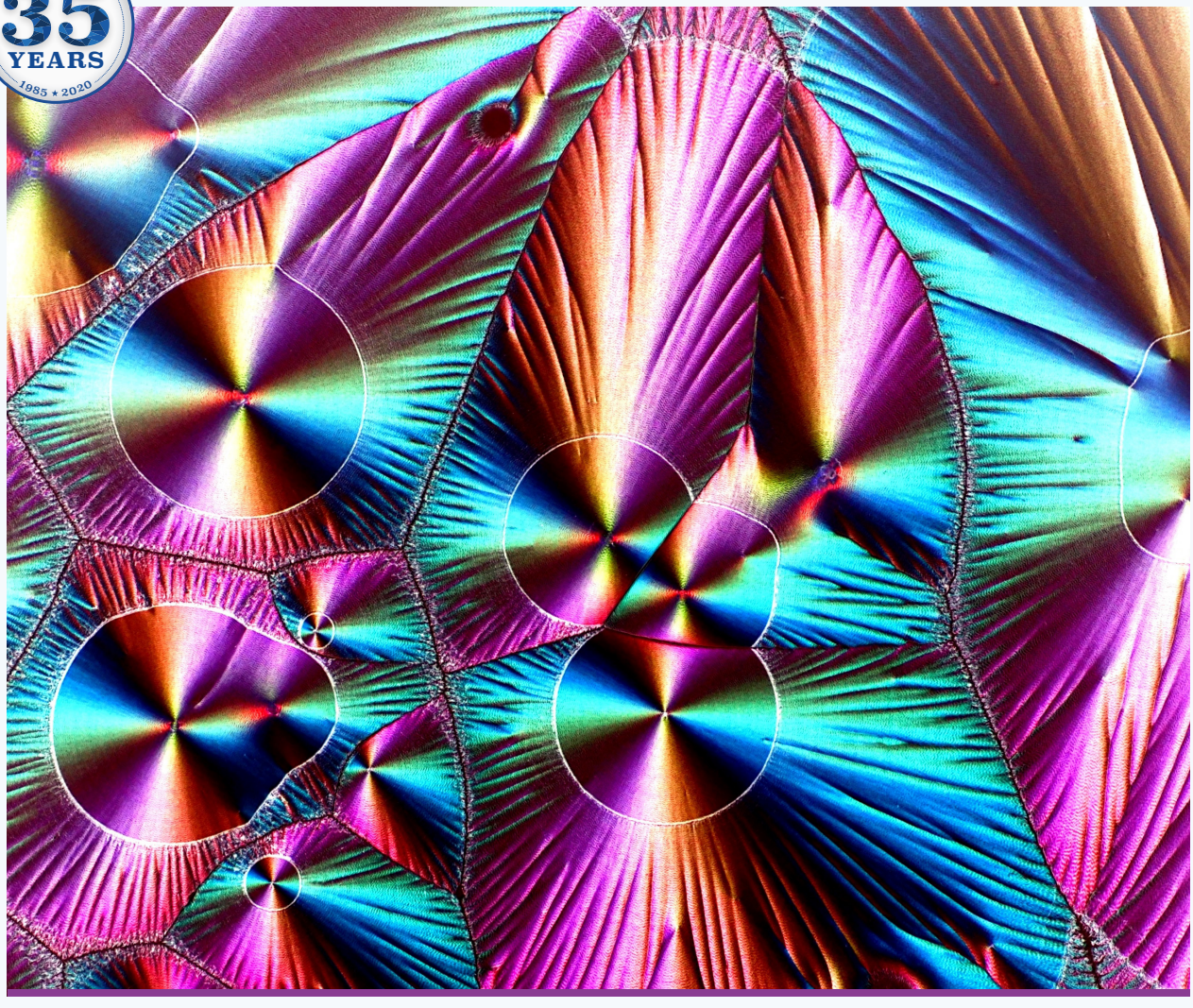

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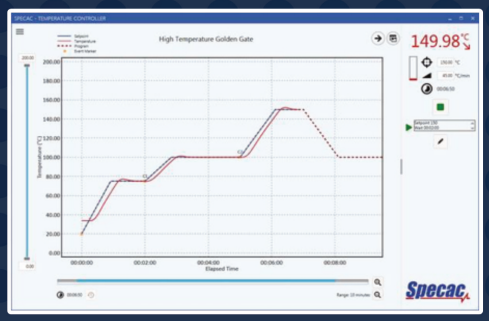

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Advances in Trace Element Solid Sample Analysis: Laser Ablation Laser Ionization TOF Mass Spectrometry (LALI-TOF-MS)

Jeffrey Williams and Jonathan Putman

The most widely used commercial techniques for solid sample analysis include laser induced breakdown spectroscopy (LIBS), arc/spark optical emission spectrometry (OES), X-ray fluorescence (XRF), and laser ablation coupled with inductively coupled plasma–mass spectrometry (LA-ICP-MS). Each technique has known limitations, including matrix suppression, diffusion and transport effects, spectral overlaps, and varying degrees of calibration challenges. Also, many laboratories determining trace impurities in solid materials are unable to reach the required limits of quantitation by direct analysis, so they must digest the samples and use a technique like ICP-MS. Recent advances in laser ablation laser ionization (LALI) have reduced many drawbacks that plague other techniques, simplifying solid sample analysis. This column examines the LALI technique coupled with time-of-flight (TOF) mass spectrometry and compares application figures of merit with other, more traditional approaches of analyzing solid materials.

Laser ablation laser ionization, coupled with time-of-flight (TOF) mass spectrometry (LALI-TOF-MS), is a brand new development that offers virtually the entire periodic table of the elements simultaneously at MS detection limits. LALI-TOF-MS has applicability to all trace element applications that require direct analysis of solid samples. LALI avoids sample digestion procedures and bypasses limitations such as matrix suppression effects, polyatomic spectral interferences, and signal instability that are exhibited in ICP-MS and other solution techniques.

At the heart of LALI-TOF-MS are two lasers; a sample chamber with ion source that is already under vacuum, and a time-TOF mass spectrometer. The dual-laser technology extracts and subsequently ionizes material in two discrete steps; first, ablation of the sample material, and then, ionization of the ablated material. The generated ions are then sampled into a TOF mass spectrometer for separation, identification, and quantification.

Historically, LALI has been referred to by numerous acronyms in the literature, including *surface analysis laser ionization* (SALI) (1,2), *laser desorption and ionization* (LDI) (3,4), *two-step laser mass spectrometry* (L2MS) (5), and *laser desorption laser post-ionization time-of-flight mass spectrometry* (LD-LPI-TOF-MS) (6). Most of the research regarding LALI was purely academic and performed between the late 1980s and early 1990s. At the time, cost and electronic limitations prohibited commercialization of LALI technology and other techniques took center stage. However, recent advances in computing technology and miniaturized, high-powered, solid-state lasers make LALI much more commercially viable today. Let's take a closer look at its fundamental principles.

Basic Principles of LALI-TOF-MS

The first step of LALI uses a focused laser beam to ablate (or desorb) material from a solid sample surface. It utilizes a neodymium-doped yttrium aluminum garnet (Nd:YAG) laser with an adjustable laser wavelength. Depending on whether the application is characterizing atoms or molecules, the laser can be set to the fourth harmonic (266 nm) or fifth harmonic (213 nm) for ablation, or the fundamental 1064 nm wavelength for desorption. In a process exactly analogous to laser ionization mass spectrometry (LIMS) and laser induced breakdown spectroscopy (LIBS), the laser

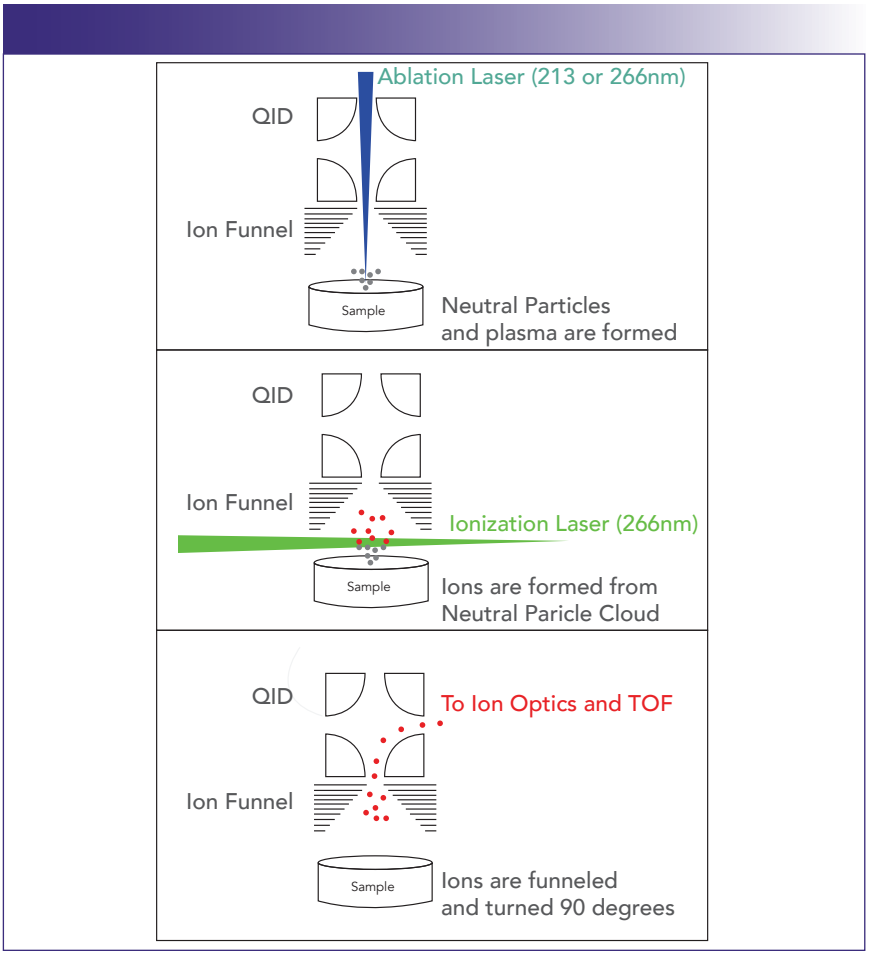

FIGURE 1: Principles of the laser ablation and ionization process.

generates an initial set of ion or electron pairs from a temporal plasma, along with a neutral particle cloud that migrates in a direction that is normal to the sample surface.

A short delay of <1 µs allows plasma extinction and the dispersion of plasma-generated ions before a second Nd:YAG laser at 266 nm is triggered for ionization. As shown in Figure 1, the ionization laser is aligned parallel to the sample surface, and its beam is focused inside the neutral particle cloud. The focused beam from the ionization laser has an energy density >109 Watt/cm^2, allowing for ionization of neutral particles via multiphoton ionization (MPI). MPI differs from resonant enhanced multiphoton ionization (REMPI), in that with MPI the laser is not tuned to a specific elemental or molecular frequency for ionization.

By ionizing elements across a wide range of ionization energies, MPI serves as a highly efficient ion source and replaces the Ar plasma of ICP instrumentation. Once ionized, an ion funnel collects and focuses the ions in a low pressure (0.2–0.3 mbar) environment. After exiting the ion funnel, a quadrupole ion deflector (QID) turns the ions 90° and directs the ion beam through an Einzel lens stack and a quadrupole to further improve the beam shape. After the transfer quadrupole, the technology is equipped with a notch quadrupole filter. For applications that require high sensitivity, the notch filter increases dynamic range by selectively reducing the signal of up to four different ion masses (typically the most abundant matrix elements). Ions are then transferred to the reflectron TOF mass spectrometer that completes the mass analysis.

Real-World Capability

To realize the real-world benefits of this technology, let's examine the following application figures of merit compared to other solid sampling approaches: All data shown have been generated on the MassBox LALI-TOF-MS instrument (Exum Instruments).

The figures we wish to examine include:

- detection capability
- matrix effects
- diffusion and transport
- spectral interferences
- ion transmission efficiency
- ability to characterize atomic and molecular species
- resolving power
- macro or micro analysis and imaging studies.

Detection Capability

Detection limits for LALI-TOF-MS are on average approximately 100–500x lower than those of either XRF or LIBS. Typical detection limits for the majority of elements by LALI are in the region of 0.01 µg/g (10 ppb) for solids, compared to approximately 1–10 µg/g (1–10 ppm) for XRF and 10–50 ppm for LIBS. The inherent limitation of both XRF and LIBS is that they rely on the generation of X-ray- and plasma-induced excitation, and, as a result, use the measurement of photons for quantification, limiting their practical detection capability, as shown in Figure 2.

LA-ICP-MS offers similar detection capability to LALI (and is slightly better for some elements) but suffers from two fundamental problems, thus limiting its suitability as a truly practical tool for a wide range of solid samples. The first major drawback of LA-ICP-MS is *elemental fractionation*, or the preferential sampling of analyte elements based on their physical size. As a result, the abundances of the ions detected after separation are not entirely representative of the composition of the original sample. Besides the ablation process itself, the transport of the aerosol particles from the ablation chamber at atmospheric pressure into the ICP are impacted by differences in gravitational settling effects between smaller and larger particles, together with vaporization, atomization, and ionization differences in the plasma (less efficient for larger

particles). In addition, transportation of ions through the interface cones, into the ion optics, and into the mass separation device are also important contributors to these fractionation effects. As a result, LA-ICP-MS often struggles to ensure that the analyte ions being measured are truly representative of the analyte elements in the bulk material being sampled, meaning that matrix matching of standards with samples is absolutely critical (7). Furthermore, LA-ICP-MS requires two separate systems from different vendors; this can be challenging to the end user to create a fluid workflow. This leads to high costs of instrument acquisition, high consumable costs, and a non-trivial amount of time from analysis to quantification. Figure 2 shows color-contoured heat maps of detection limits for LALI-TOF-MS (top) compared to LA-ICP-MS, XRF, and LIBS (bottom). The darkest colors represent the lowest limits of detection and clearly show that LALI offers the best detection capability across the periodic table.

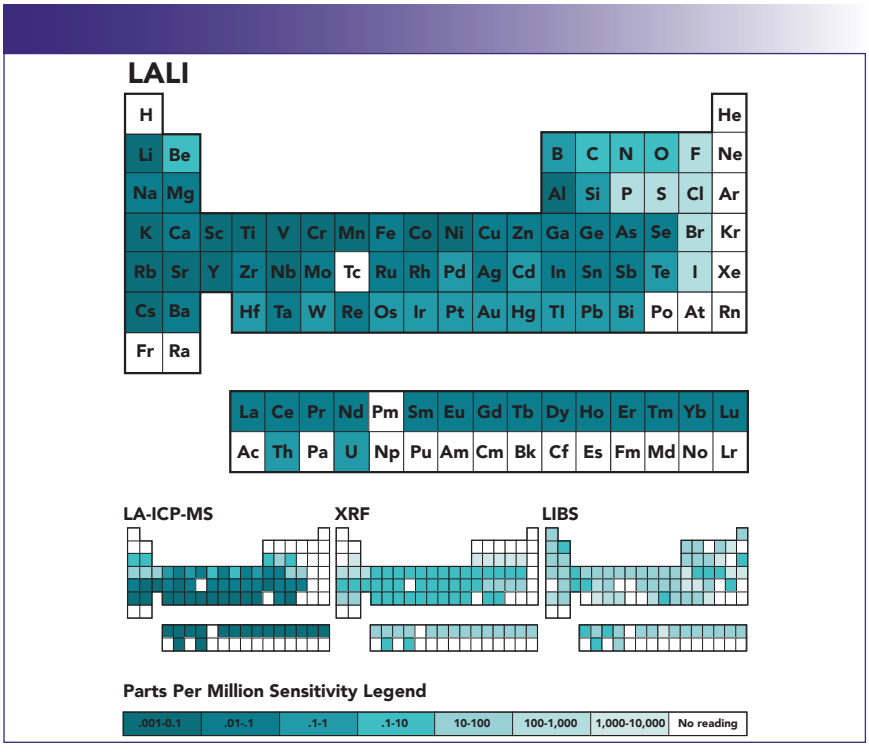

FIGURE 2: Detection limits of LALI-TOF-MS compared to LA-ICPMS, XRF and LIBS.

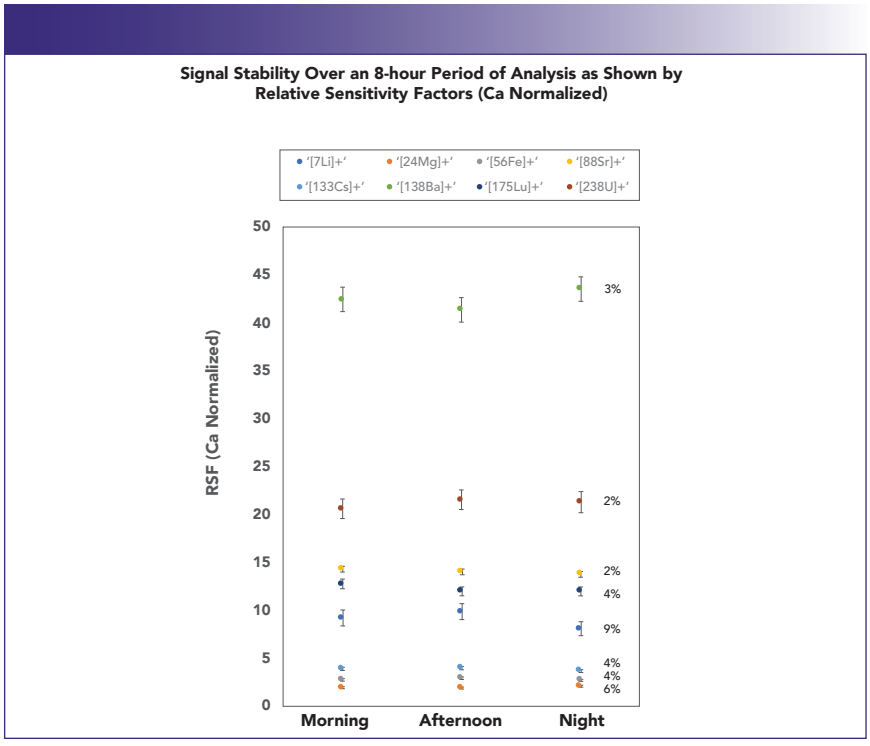

FIGURE 3: Long-term stability of a suite of trace elements in NIST 610 standard reference glass over an 8-h period.

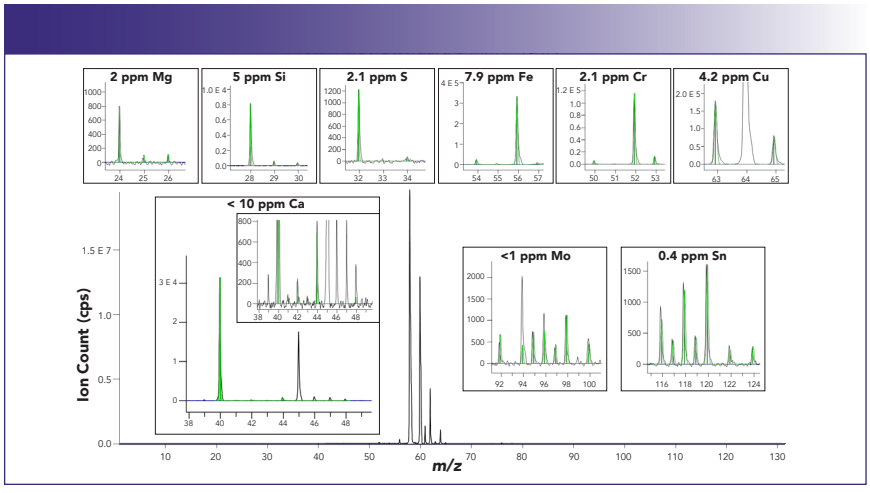

FIGURE 4: Metal alloy standard IARM-191A: Detection of ppm levels of Mg, Si, S, Fe, Cr, Cu, Ca, Mo, and Sn in a high purity nickel CRM showing no spectral overlaps from Ar-, O-, N-, or C-based polyatomic-isobaric interferences as demonstrated by the theoretical isotopic distributions represented by the green traces.

Matrix Effects

In XRF, the sample is irradiated with a beam of high-energy X-rays. As the excited electrons in the atom fall back to a ground state, they emit secondary X-rays that are characteristic of those elements present in the sample. Its inherent weakness lies in the fact that because the generation of secondary X-rays is dependent on the analyte–matrix bond, matrix-matched standards are a critical requirement for reliable quantification. So, for applications that require multielement measurements across a variety of different matrices, this is a well-recognized limitation of the XRF technique. On the other hand, LIBS uses plasma-generated photons produced by a combination of excitation and ionization from the laser, which are significantly affected by the matrix elements. LALI, however, has more efficient ionization and significantly lower matrix effects, making quantification more straightforward. LALI's strength over LIBS is that the source ionizes gas-phase particles within the neutral particle cloud, instead of relying on plasma generated ions during ablation. As a result, the LALI particles in the neutral cloud are significantly less variable across different matrices. Ionization of neutral cloud material also results in stoichiometric accuracy, enabling quantification of a variety of sample matrices without the need for matrix-matched standards.

Diffusion and Transport of Ions

Another major advantage of the LALI design is that ionization occurs under vacuum in the sample chamber. It is a completely static system, held at high-vacuum (~10^{-7} mbar) in the TOF, and a pressure gradient to ~10^{-4} mbar in quadrupoles and the ion optics. The pressure in the LALI sample chamber is maintained at ~0.2–0.3 mbar with an inert helium cooling gas system. The low pressure of the ion source results in a significant improvement in sensitivity, because it greatly reduces losses associated with gas transport from atmospheric pressure to a vacuum system.

The removal of the plasma source also has the advantage that thermal emission of contaminant ions from the cones or injector is eliminated, greatly improving the ability to determine many of the volatile elements at both low and high masses, including Na (mass 23) and Pb (masses 201, 206, 207, and 208). Additionally, without a plasma source or any carrier gas, LALI does not rely on components with dynamic fluctuations, thus leading to long-term signal stability without requiring regular instrument tuning and calibration. Figure 3 shows the long-term stability of a suite of trace elements in a NIST 610 standard reference glass over a period of 8 h, with the precision (% RSD) of multiple measurements. Note that each of the three sets of data points (morning, afternoon, and night) represents an average of 1000 scans.

Spectral Interferences

Without an ICP source, the technique does not require a carrier gas, eliminating all polyatomic molecular interferences derived from argon. In addition, because there is very little opportunity for air entrainment inside the ionization chamber, all oxygen, nitrogen, and carbon-based polyatomic and isobaric interferences are drastically reduced. Elimination of these ionic species significantly improves the detection for a whole host of elements, including Si, S, Ca, Mg, Si, Cr, and Fe, which are traditionally problematic for ICP-MS. This is exemplified in Figure 4, which show a 0–130 amu scan of a high purity nickel certified reference material (IARM-191A, Analytical Reference Materials, Intl.). The major isotopes of nickel at masses 58, 60, 61, 62, and 64 amu are shown in the center of the scan, while zoomed sections are shown in the boxes. It can be seen that spectral peaks for the different isotopes of Mg, Si, S, Fe, Cr, Cu, Ca, Mo, and Sn are clearly being detected and measured at the low ppm level. It should also be emphasized that using an ICP-MS instrument, either as a solution technique or coupled with a laser ablation system, there would be large spectral overlaps from $^{12}C^{12}C$ on ^{24}Mg; $^{14}N^{14}N$ on ^{28}Si, $^{16}O^{16}$ on ^{32}S; $^{40}Ar^{16}O$ on ^{56}Fe, $^{40}Ar^{12}C$ on ^{52}Cr, and ^{40}Ar on ^{40}Ca. The green traces, which represent theoretical isotopic distributions, closely match the experimental results across the entire mass range, indicating that no such spectral overlaps are present.

To emphasize the purity of the elemental spectral fingerprints across the entire mass range, Figures 5a and 5b show a LALI mass spectrum of a NIST 610 standard reference glass. Figure 5a exemplifies a suite of transition elements in the spectral region 0–90 amu, free of the most common polyatomic and isobaric interferences, while Figure 5b shows some rare earth elements in the spectral region 90–220 amu, where doubly charged interferences are commonly observed. Theoretical isotopic distributions are shown in green.

Ion Transport Efficiency

LALI also provides considerable improvements in transmission efficiency of an ion beam compared to techniques that generate ions at atmospheric pressure. For example, ions generated by the plasma discharge of an ICP-MS instrument at atmospheric pressure are generally transferred in several stages before reaching the high-vacuum mass analyzer. Each stage transition of cones and/or lenses removes a significant portion of ions. For instance, LA–ICP–MS has a very high ionization efficiency for elements with a first ionization potential (FIP) less than 8 eV, but only ~1 in every 10^5–10^6 ions reach the detector (~0.01–0.001% transmission efficiency). The LALI source is already under vacuum, so it does not suffer from transmission loss going from atmospheric pressure to vacuum. Removing the atmospheric or vacuum interface greatly improves transmission efficiency, allows for higher sensitivity, and further reduces matrix effects by removing plasma-ion spatial interaction effects.

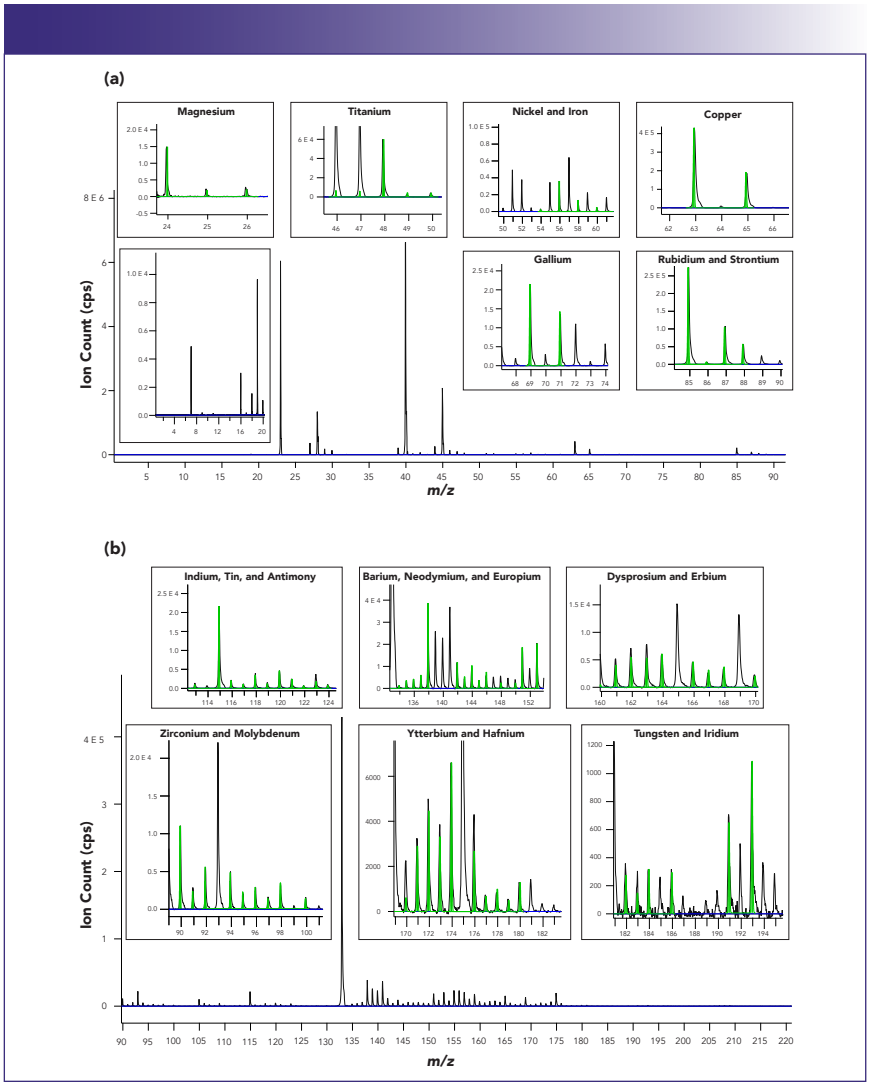

FIGURE 5: (a) LALI spectral scan (0–90 amu) of NIST 610 standard reference glass, with zoomed regions of specific elements highlighted; (b) LALI mass spectrum (90–220 amu) of NIST 610 standard glass, with zoomed regions of specific elements highlighted.

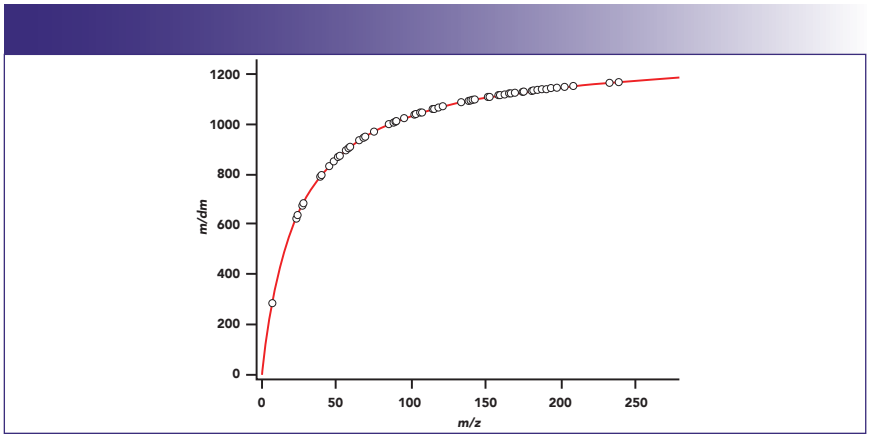

FIGURE 6: Plot of mass resolving power (m/dm) against mass (*m/z*) for the TOF mass spectrometer used for elemental analysis.

Identification of Atomic and Molecular Species

LALI is capable of analyzing both inorganic and organic species, which is difficult to carry out with other techniques that suffer from the problems previously discussed (8). The ability to analyze organic compounds by LALI has been studied by many groups for applications including planetary missions and crude oil analysis (6,9). The analysis of organics utilizes the infrared (IR) component of the Nd:YAG laser (1064 nm). The intense IR pulse flash heats the sample (10^8 K/s) to desorb intact material from the sample surface (10). Following desorption, organic compounds are ionized via MPI, using the secondary ionization laser as previously described. The ability to analyze both organics and inorganics in the same analytical run enables mapping (or bulk characterization) of both in the same sample almost simultaneously after a quick mode switch. To enable accurate assessment and interpretation of molecular species, an optional high resolution TOF mass spectrometer with a resolving power of up to 14,000 is available.

Resolving Power

LALI–TOF-MS is suited to many application areas by customizing the configuration of the mass spectrometer, based on the spectral demands of the analysis. Under normal conditions for carrying elemental analysis, the resolving power (m/dm) of the TOF mass spectrometer is in the order of 700–1100 (the range for quadrupole MS is typically 400–500). However, for characterizing molecular species, the resolving power can be increased from 7000 up to 14,000. Figure 6 is a plot of resolving power (as m/dm) against mass (*m/z*) for the typical configuration used for trace element analysis.

To demonstrate the practical benefits of resolving power, a spectral scan of five barium isotopes at 138, 137, 136, 135, and 134 amu using a resolving power of 750 is exemplified in Figure 7, showing the clean separation and the isotopic purity of the Ba isotopes (theoretical distribution of the isotopes is shown in green). A comparison of experimental vs. theoretical abundances for each of the isotopes

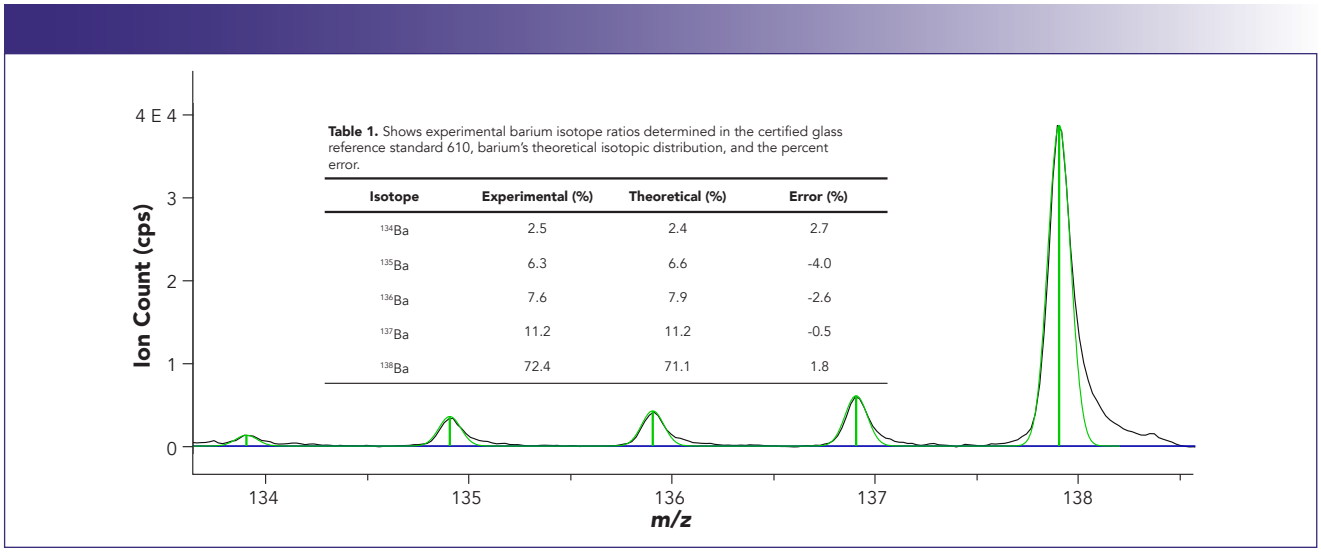

Table 1. Shows experimental barium isotope ratios determined in the certified glass reference standard 610, barium's theoretical isotopic distribution, and the percent error.

Isotope	Experimental (%)	Theoretical (%)	Error (%)
^{134}Ba	2.5	2.4	2.7
^{135}Ba	6.3	6.6	-4.0
^{136}Ba	7.6	7.9	-2.6
^{137}Ba	11.2	11.2	-0.5
^{138}Ba	72.4	71.1	1.8

FIGURE 7: A spectral scan of five barium isotopes (138, 137, 136, 135, and 134 amu), using a resolving power of 750, showing good agreement between experimental and theoretical abundances.

is also shown, which demonstrates very good agreement, within experimental error.

Macro and Micro Analysis and Imaging Applications

This technology is well suited for both macro and micro analysis, together with laser imaging studies. This is exemplified in Figure 8, which shows the sample chamber opening to allow the sample tray to be loaded.

A macro-camera then opens to take a high-precision, spatially located picture. After the sample chamber door closes the chamber begins to pump down to vacuum, and the high-resolution image from the macro-camera is loaded onto the touch screen interface. The macro-image is used to enable navigation around the samples, as shown in Figure 9. Moving back and forth on the screen physically moves the sample stage within the chamber, and aligns the desired area properly with the lasers. "Pinching" on the image zooms in and switches to a live microscopy image that allows precision when choosing an area to analyze. From the live view, spots, lines, or rasters for maps are chosen. After selecting the type and number of sampling areas, analysis and data processing are automated, and all that remains is to interpret the results. This capability is well-suited for microanalysis of small surface inclusions, depth profiling analysis for coating thickness, or two-dimensional, high-spatial-resolution, multi-elemental mapping, rapidly becoming an important research tool in the field of geological, biological and medical imaging studies (11).

Summary

LALI-TOF-MS provides high specificity and high sensitivity quantitative analysis for both bulk and micro analysis, together with elemental and chemical mapping, without the need for complex quantification schemes or matrix-matched standard materials. The technique's simple design enables field portability, and its easy-to-use, intuitive interface makes personnel and training requirements very straightforward.

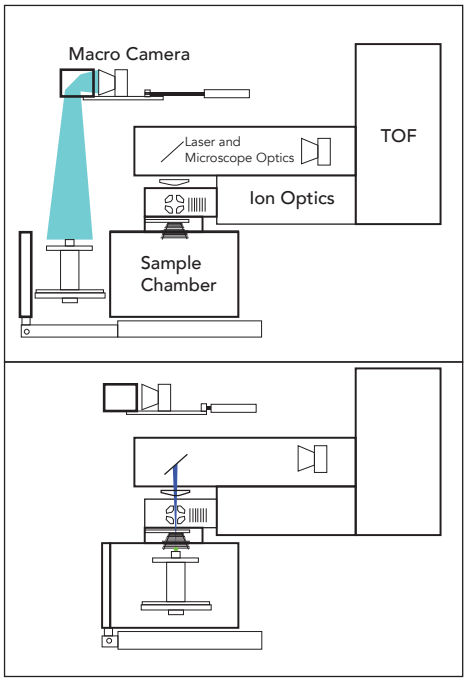

FIGURE 8: Schematic of sample loading for macro imaging using a LALI source.

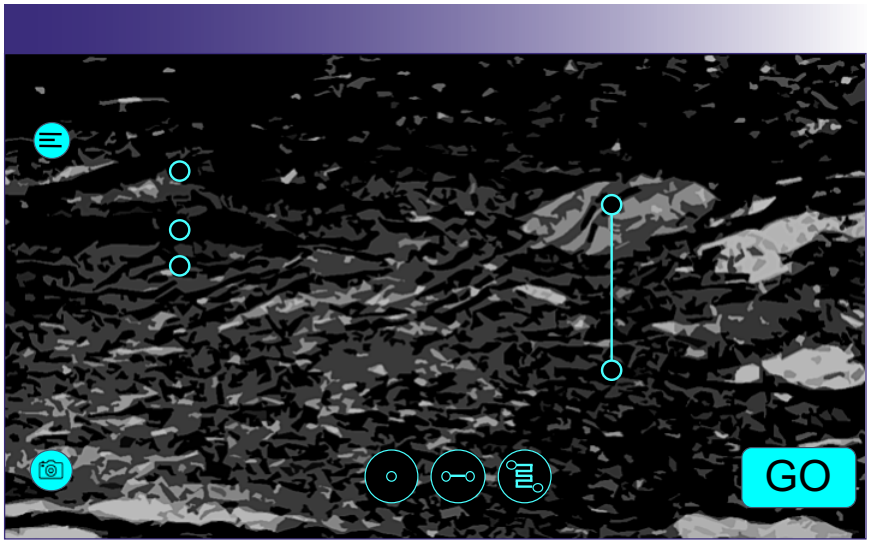

FIGURE 9: The macro-image is used to enable navigation around the sample to select regions for further micro investigation.

Together, these factors open a wide range of potential inorganic and organic application areas. As a result, this emerging technology is expected to have a large impact in the field of geological, metallurgical, petrochemical, agronomy, agricultural, biological, and cannabis studies.

References

(1) C.H. Becker and K.T. Gillen, *J. Opt. Soc. Am. B* **2,** 1438 (1985).

(2) C.H. Becker and K.T. Gillen, *Anal. Chem.* **56,** 1671–1674 (1984).

(3) G.R. Kinsel and D.H. Russell, *J. Am. Soc. Mass Specrom.* **6,** 619–626 (1995).

(4) S.A. Getty et al., *Rapid Commun. Mass Spectrom.* **26,** 2786–2790 (2012).

(5) P. Hurtado, F. Gamez, and B. Martinez-Haya, *Energy Fuels* **24,** 6067–6073 (2010).

(6) H. Sabbah et al., *Energy Fuels* **26,** 3521–3526 (2012).

(7) A. Limbeck et. al., *Anal. Bioanal. Chem.* **407**(22), 6593–6617 (2015).

(8) B. Schueler and R.W. Odom, *J. App.Phys.* **61,** 4652–4661 (1987).

(9) J.H. Hahn, R. Zenobi, and R.N. Zare, *J. Amer. Chem. Soc.* **109,** 2842–2843 (1987).

(10) L. V. Vaeck and R. Gijbels, *J. Anal. Chem.* **337,** 743–754 (1990).

(11) Y. Bussweiler, O. Borovinskaya, and M. Tanner, *Spectroscopy* **32**(5), 14–20 (2017).

ABOUT THE AUTHORS

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Organic Nitrogen Compounds IX: Urethanes and Diisocyanates

Brian C. Smith

The urethane functional group is found almost exclusively in polymer form, known as *polyurethanes*. These ubiquitous polymers make urethanes an economically important functional group. Urethanes are made using diisocyanates. How to identify diisocyanates, and distinguishing among different urethane types using infrared spectroscopy, are explained in this installment of the column.

The urethane functional group is found almost exclusively in polymer form, known as *polyurethanes*. These ubiquitous polymers are used as wood finishes and make up polyurethane foam, also known as foam rubber. The structural framework of a urethane is shown in Figure 1.

Note that this functional group contains a carbonyl bond with an oxygen atom and nitrogen atom attached to it. The latter is why urethanes are included in this series on organic nitrogen compounds. On the left-hand side of Figure 1, the urethane looks like an ester because of the O-C=O linkage (1), but on the right-hand side of Figure 1, the N-C=O linkage looks like an amide (2,3). As we will see, the infrared spectra of urethanes combine features of both esters and amides.

Like amides, urethanes are denoted as *primary* if one carbon and two hydrogens are attached to the nitrogen atom, as *secondary* if two carbon atoms and one hydrogen atom are attached to the nitrogen, and as *tertiary* if three carbon atoms are attached to the nitrogen. Figure 1 shows the structure of a secondary urethane. Note that it contains two C-N bonds and one N-H bond.

Polyurethanes are made by reacting alcohols with a functional group called a *diisocyanate*. The structural framework of a diisocyanate is seen in Figure 2.

Note that a diisocyanate contains two isocyanate -N=C=O linkages, hence the "di" in the name. A molecule with one -N=C=O unit would simply be called an *isocyanate*. When urethanes and alcohols are polymerized to make polyurethanes, there can be isocyanate end groups that occasionally appear in the spectra of polyurethanes.

The Infrared Spectra of Diisocyanates

The infrared spectrum of a diisocyanate is shown in Figure 3.

Note that the spectrum is dominated by the peak labeled A at 2277 cm^{-1} (assume all peak positions are in wavenumbers going forward, even if not labeled as such). This peak is due to the asymmetric stretch of the -N=C=O group, which normally falls from 2280 to 2240. This peak is the perfect example of a group wavenumber, because it is intense and shows up in a part of the spectrum where very few other functional groups absorb (5). Throughout the over 30 installments of this column, you may have noticed that most of the time we focus our attention from 3500 to 2800, and

TABLE I: Group wavenumbers for diisocyanates and urethanes

Vibration	Wavenumbers (cm^{-1})
Isocyanate asymmetric N=C=O stretch	2280–2240
Primary urethane NH_2 stretches	3450–3400, 3240–3200
Primary urethane C=O	1740–1730
Primary urethane NH_2 wag	1630–1610
Secondary urethane N-H stretch	3340–3250
Secondary urethane C=O	1740–1705, 1 or 2 Peaks
Secondary urethane N-H bend	1540–1520
Tertiary urethane C=O	1690–1680
Urethane C-O stretch	1265–1200

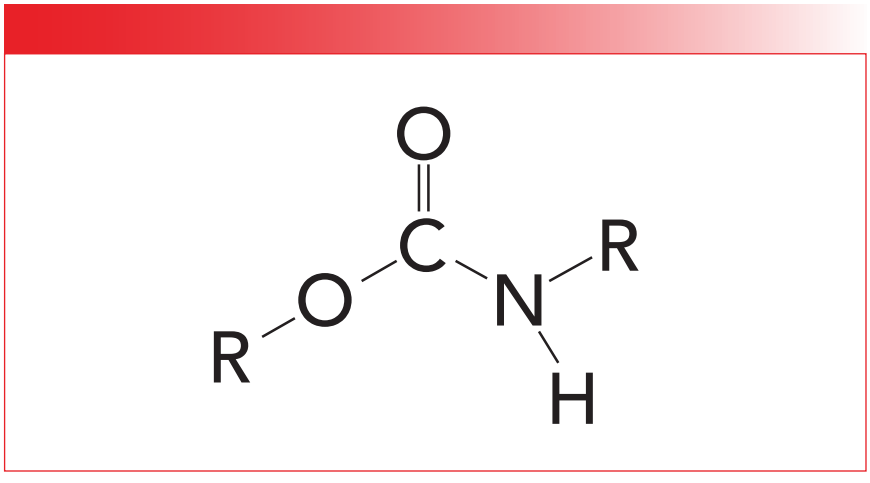


FIGURE 1: The structural framework of a secondary urethane.

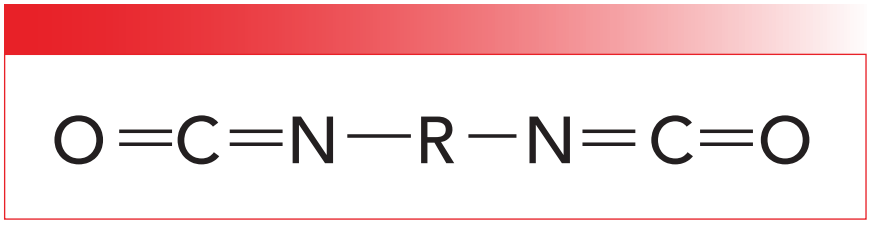


FIGURE 2: The structural framework of the diisocyanate functional group.

from 2000 to 400. That is because very few functional groups absorb between 2800 and 2000. The only other infrared peak we have seen that absorbs near diisocyanates is the C≡C stretch of disubstituted alkynes, which fall from 2260 to 2190 (6). These two functional groups are easily distinguished, because the diisocyanate -N=C=O asymmetric stretching peak is broader and stronger than a typical C≡C stretch. This is because of the high polarity of the -N=C=O group compared to that of an alkyne triple bond (7). The strength and unusual position of the -N=C=O stretching peak are why it sometimes appears in polyurethane spectra, even though it is in low concentration.

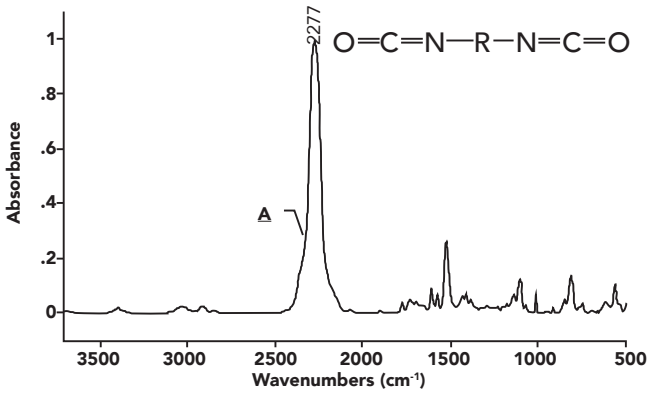
The Infrared Spectra of Urethanes

Based on the structural framework of urethanes shown in Figure 1, we can predict to a point what urethane spectra will look like. Primary and secondary urethanes contain N-H bonds, and so have N-H stretches that are medium in width and intensity, and fall in the same wavenumber range as the N-H stretching peaks of amides and amines (2–4). The C=O bond in urethanes means there should be a strong C=O stretching peak (8) from around 1700, and the C-O bond means there should be a strong peak between 1300 and 1000 (9).

The infrared spectra of primary urethanes behave as expected. Their asymmetric and symmetric NH_2 stretches are found from 3450 to 3400 and 3240 to 3200, respectively. Primary urethanes have two NH stretching peaks, as do primary amines and amides (2–4), because, in all these cases, the primary nitrogen contains two N-H bonds, hence two N-H stretching peaks (3). The carbonyl stretch of primary urethanes falls at 1740 to 1730, and there is an NH_2 scissors (in-plane bending) peak from 1630 to 1610.

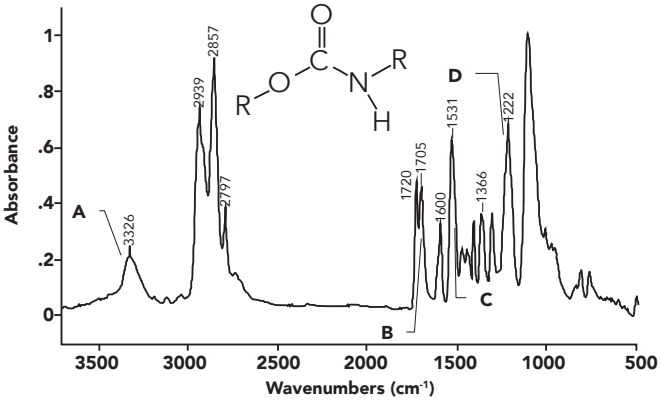
Unfortunately, the C=O stretching peak of primary urethanes falls in the same region as other carbonyl-containing functional groups, such as ketones, aldehydes, esters, and carboxylic acids (8,9). However, these functional groups do not contain nitrogen, hence there are no N-H stretching peaks, making distinguishing primary urethanes from these compounds easy. But primary amides have two NH_2 stretches, and a C=O stretch (3), as do primary urethanes. Fortunately, the primary urethane C=O stretch is at 1740 to 1730, whereas, for primary amides, it falls from 1680 to 1630 (10). This difference in C=O stretching peak position means primary amides and urethanes can be distinguished from each other. The diagnostic group wavenumber pattern, then, for primary urethanes is two NH stretching peaks, a C=O peak around 1730, and an NH_2 scissors peak.

The infrared spectrum of a secondary urethane, a "polyurethane/polyether



A	2277	N=C=O Asymmetric stretch

FIGURE 3: The infrared spectrum of a diisocyanate.



A	3326	N-H Stretch
B	1720,1705	C=O Stretch
C	1531	N-H Bend
D	1222	C-O Stretch

FIGURE 4: The infrared spectrum of a polyurethane/polyether foam.

foam," better known as foam rubber, is seen in Figure 4.

Because this polymer is a secondary urethane, as seen in the figure, it has a single N-H bond, and, hence, a secondary nitrogen. The spectral signature of a secondary nitrogen, as we saw for secondary amides and amines (2–4), is a single N-H stretching peak. In Figure 4, this peak is labeled A at 3326. In general, for secondary urethanes, this peak falls from 3340 to 3250. Note that the NH stretching peak in Figure 4 is of medium intensity and height, consistent with many of the other NH stretches we have seen (11).

The carbonyl stretch in Figure 4 labeled B is split, with peaks at 1720 and 1705. In the past, a double carbonyl stretch like this indicated the presence of two separate carbonyl bonds in a functional group, such as for acid anhydrides (12) and imides (13). However, this is clearly not the case here; urethanes do not contain two carbonyl bonds. The cause of this split carbonyl peak is that some urethane C=O groups engage in hydrogen bonding, whereas others don't. The 1720 peak is from non-hy-

Solution to the Last Infrared Spectral Interpretation Challenge

The spectrum from the last interpretation challenge is seen in Figure i.

As we work our way from left to right across this spectrum, the first peak we encounter is at 3043. We have learned that peaks between 3100 and 3000 are typically the C-H stretch of unsaturated carbons (15). However, this peak by itself cannot help us distinguish between the two most common unsaturated carbon types, alkenes or benzene rings. Alkenes have a C=C stretching peak from 1680 to 1630 (15), but, given that there are no peaks in this region in this spectrum, we can rule out an alkene. Benzene rings have ring mode peaks that are sharp, and appear from 1630 to 1400 (16). The sharp peak at 1500 can be assigned as a ring mode, indicating we have a benzene ring present.

The most notable feature in Figure i is the pair of peaks at 1777 and 1726. Given their position and intensity, they are C=O stretching vibrations (8). The fact that there are two carbonyl stretching peaks indicates there may be a functional group present with two C=O bonds in it. Acid anhydrides are a possibility here, because we have seen that their spectra possess a double carbonyl stretching peak (12). However, the acid anhydride functional group also contains a C-O bond, and, hence, should have a strong C-O stretching peak between 1060 and 1035. There are no strong peaks in this region, meaning this is not an acid anhydride.

We saw last time (13) that cyclic imides have a double carbonyl stretch with peaks at 1790 to 1735 and 1750 to 1680. The spectrum in Figure i has peaks at 1777 and 1726, consistent with there being a cyclic imide present.

Now, some imides have an N-H bond, and, hence, an NH stretching peak at 3200±50 (13). The absence of an NH stretch here means there is not an NH bond, but, more than likely, a C-N bond in the imide functional group. Note that the caption in Figure i says the sample is a fiber. This means the sample is a polymer, and we probably have a polyimide where the repeat units connect through the nitrogen in the imide functional group, explaining the lack of an NH stretch.

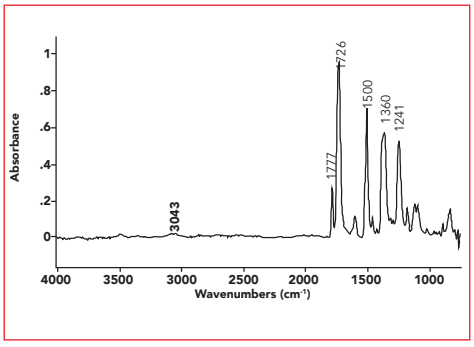


Figure i: The infrared spectrum of a fiber.

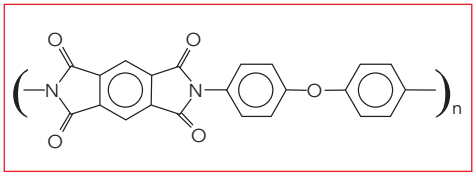


FIGURE ii: The chemical structure of Kapton, the answer to this Interpretation Challenge.

I am afraid this is as far as we can push this analysis. What we know is that we have a cyclic aromatic polyimide. The most common material fitting this description has the trade name Kapton, or the chemical name poly(4,4′-oxydiphenylene-pyromellitimide). Given this name, you can see why we will simply call this material Kapton. The chemical structure of Kapton is seen in Figure ii.

Note there is also an aromatic ether in this structure, hence the C-O stretch in Figure i at 1241 (14).

Quiz Section

Your Next Infrared Spectral Interpretation Challenge

The interpretation challenge is currently is on spring break. It will return in a future column.

drogen bonded, or "unassociated," carbonyls, whereas the 1705 peak is from the hydrogen bonded, or "associated," carbonyl groups (10). We have already studied the effects of hydrogen bonding on peaks, such as for alcohols (9). The tendency for peaks upon hydrogen bonding is to broaden and move to lower wavenumbers, as we have seen here.

The peak labeled C in Figure 4 at 1531 is the in-plane N-H bend of a secondary urethane. In general, this peak falls from 1540 to 1520. Secondary amides also have a peak from the same vibration in the same place (3). However, secondary amide C=O stretches fall from 1680 to 1630, whereas, for secondary urethanes, this peak falls from 1740 to 1705, higher than in secondary amides, allowing us to distinguish between secondary urethanes and amides.

The diagnostic group wavenumber pattern then for secondary urethanes is a single N-H stretch, a carbonyl stretch from 1740 to 1705, and an N-H in-plane bend from 1540 to 1520. Primary and secondary urethanes can be distinguished, because the former has two NH stretching peaks, whereas the latter has one.

A further examination of Figure 1 shows that urethanes have a C-O

bond, and we have learned in general that C-O stretching peaks are intense and fall from 1300 to 1000 (9). The peak labeled D at 1222 in Figure 4 is a urethane C-O stretch. The C-O stretch for all urethanes falls from 1250 to 1200 (10). There is a large peak at ~1050 in Figure 4 that is not labeled. It is from the C-O stretch of the ether groups (14) in this particular polyurethane/polyether foam.

Tertiary urethanes contain no NH bonds, hence they have no NH stretching or bending peaks. Their only useful group wavenumber is their C=O stretch from 1690 to 1680 (10), which also overlaps with amides. Thus, tertiary urethanes, like tertiary amines and amides (2–4) are a functional group that is hard to distinguish by infrared spectroscopy.

A summary of the group wavenumbers discussed in this column is seen in Table I.

Conclusions

Urethanes are often made into polyurethanes by reaction with diisocyanates. Diisocyanates have a strong and uniquely positioned -N=C=O asymmetric stretching peak from 2280 to 2240. Like amides and amines, urethanes can be classified as primary, secondary, and tertiary, based on the number of C-N and N-H bonds. Primary urethanes exhibit two NH stretches, a C=O stretch, and an NH_2 scissoring vibration. Secondary urethanes have one NH stretch, a C=O stretch, and an NH in plane bend. Tertiary urethanes are difficult to discern by infrared spectroscopy.

References

(1) B.C. Smith, *Spectroscopy* **33**(7), 20–23 (2018).
(2) B.C. Smith, *Spectroscopy* **34**(11), 30–33 (2019).
(3) B.C. Smith, *Spectroscopy* **35**(1), 10–15 (2020).
(4) B.C. Smith, *Spectroscopy* **34**(3), 22–25 (2019).
(5) B.C. Smith, *Spectroscopy* **31**(1), 14–21 (2016).
(6) B.C. Smith, *Spectroscopy* **32**(7), 18–24 (2017).
(7) B.C. Smith, *Spectroscopy* **30**(1), 16–23 (2015).
(8) B.C. Smith, *Spectroscopy* **32**(9), 31–36 (2017).
(9) B.C. Smith, *Spectroscopy* **32**(1), 14–21 (2017).
(10) G. Socrates, *Infrared and Raman Characteristic Group Frequencies* (Wiley, New York, New York, 3rd Ed., 2001).
(11) B.C. Smith, *Spectroscopy* **34**(1), 10–15 (2019).
(12) B.C. Smith, *Spectroscopy* **33**(3), 16–20 (2018).
(13) B.C. Smith, *Spectroscopy* **35**(3), 26–30 (2020).
(14) B.C. Smith, *Spectroscopy* **32**(5), 22–26 (2017).
(15) B.C. Smith, *Spectroscopy* **31**(11), 28–34 (2016).
(16) B.C. Smith, *Spectroscopy* **31**(3), 34–37 (2016).

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The Effect of High Pressure on Ascorbic Acid Structure

Jingkai Bi, Yujie Shang, Yue Zhao, Dongfei Li, and Mi Zhou

In situ high-pressure Raman measurement of ascorbic acid has been conducted in the pressure range of ambient pressure to 14 GPa. A phase transition occurs at 3.8G Pa, and, at the pressure of 3.8 GPa, a small C=O band appears at 1767 cm^{-1}, and the intensity increased with further compression. Furthermore, as the pressure increases, the crystal symmetry of ascorbic acid becomes lower.

Ascorbic acid, also known as vitamin C, is an acidic and strongly reducing polyol containing six carbon atoms. It is a colorless and odorless flake crystal, soluble in water, but insoluble in fat solvents (1,2). Ascorbic acid is easily oxidized to dehydrogenated vitamin C, but it is stable in an acidic environment. It is easily oxidized by oxygen, and is susceptible to temperature, pH, copper ions, iron ions, and light (3). Ascorbic acid is widely found in fresh vegetables and fruits, as well as in other foods. It is one of the important nutrients for human nutrition. If the body lacks ascorbic acid, it can cause scurvy, characterized by bleeding in the skin and gums (4,5). In addition, it is a neuromodulator, and is used by neurons in many different functions and enzymatic reactions (6–8). Due to its high reactivity to oxygen, ascorbic acid has received extensive attention related to the prevention and treatment of cancer (9–13).

In the past two decades, high-pressure in situ Raman spectroscopy, using diamond anvil cell technology, has become one of the important means to study molecular structure and properties under high pressure (14–20). We can study the changes in material structure and electron orbital changes through Raman spectroscopy (21–26).

Pressure is an effective thermodynamic parameter, and is considered a powerful tool for studying the detailed structure and physical and chemical properties of matter. Pressure can effectively change the lattice structure, and therefore shorten the distance between atoms—this affects the nature of chemical bonds between molecules, molecular conformation, crystal structure, and solid stability (27–30). Pressure-induced phase transition is a common phenomenon in high-pressure science. To date, a high-pressure Raman study of ascorbic acid has not been reported.

Experiment

The ascorbic acid used in this experiment was purchased from Sigma Aldrich, and was used without purification. The high-pressure cell used in the experiment is a symmetric diamond anvil cell (DAC). The DAC has two diamonds with 500 µm culet size. A T301 (thickness 250 µm) steel gasket was used as a sealing device for generating high-pressure. Ruby powder, having a diameter of about 12 µm, was used as an internal standard to calibrate and convey the pressure in the cavity. The ruby fluorescent line R1 (at a wavelength of 694.2 nm) linearly moves as the pressure increases (31). No additional pressure-transmitting medium was used in this experiment.

Raman spectra were measured using a Renishaw instrument via confocal Raman spectroscopy. The excitation source was

a 514.5 nm Argon Particle Laser (Spectra Physics 160M). Backward Raman scattering was measured with a 50× objective lens. The laser power used was 10 mW. The accumulation time for the measurement was typically 60 s. All of the experiments were carried out at constant room temperature (~21 °C).

Results and Discussion

Raman Spectra of Ascorbic Acid

Ascorbic acid crystal belongs to the monoclinic crystal system, and its space group is P21 (32,33). Figures 1 and 2 show the crystal structure and Raman spectrum of ascorbic acid, respectively, in a normal-pressure environment. The Raman spectrum of ascorbic acid is consistent with what Singh and associates have reported (8). The strong Raman scattering lines located at 1124, 1651, 1664, and 2915 cm^{-1} are assigned to C-O bending, C=C stretching, and C-H stretching, respectively. Peaks at 562 and 583 cm^{-1} are attributed to be OH out-of-plane deformation and C=C ring stretching mode, respectively. Detailed Raman vibrational assignments are given in Table I.

High-Pressure Raman Spectroscopy of Ascorbic Acid

Figure 3 shows the high-pressure Raman spectra of ascorbic acid. It can be seen that as the pressure increases the bandwidth of most Raman bands will gradually widen. The Raman peaks shift to a higher wavenumber region. This is because, as the pressure is gradually increased, the distance between atoms decreases, and the force constant of the valence bonds increases, so that the vibration frequency increases. Figure 3 shows the Raman spectra of ascorbic acid recorded at selected pressure for the 100–3200 cm^{-1} spectral region. Raman spectra below 100 cm^{-1} cannot be observed, due to the notch filter in use. In addition, it is difficult to identify the Raman peaks at around 1340 cm^{-1}, due to the first-order Raman peaks of the diamond cell. Furthermore, as can be seen from Figure 3, with the increase of pressure, the vibration intensity of the Raman band at 583 is enhanced. This may be due to the compression of the C=C ring, and the change in the dihedral angle of the OH outside the ring. And at the pressure of about 3.8 GPa, a weak C=O stretching band appears at 1767 cm^{-1}. Further compression will result in a gradual increase in the intensity of this band—possibly the result of the activation of the silent mode, due to changes in molecular symmetry (23).

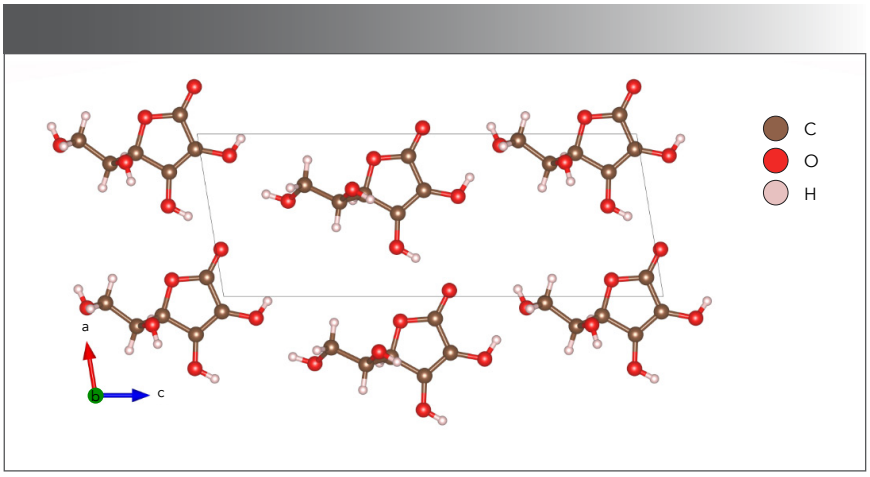

FIGURE 1: Crystal structure of ascorbic acid.

TABLE I: Raman frequency (cm^{-1}) assignments of ascorbic acid (5).

Raman Band	Assignment
3000	C-H stretching
2915	C-H stretching
1746	C=O stretching
1664	C=C stretching
1651	C=C stretching
1487	C-H bending
1293	C-O-H bending(twisting)
1253	C-O-H bending(twisting)
1124	C-O-C stretching, ring deformation
1024	C-O-H bending
868	C-C ring stretching
818	C-C ring stretching
693	OH out-of-plane deformation/C-C ring stretching
625	OH out-of-plane deformation/C-C ring stretching
583	OH out-of-plane deformation/C-C ring stretching
562	OH out-of-plane deformation/C-C ring stretching
444	C-O in-plane deformation
220	C-OH bending

Frequency–Pressure Relationship of Ascorbic Acid

In general, the Raman frequency pressure relationship can provide useful information about the crystal structure at high pressure. In addition to the disappearance of the original peaks and the appearance of new peaks, the frequency–pressure relationship is also an important indicator of the pressure-induced phase transition (34–35). As can be seen in Figure 4, with an increase of pressure, the relationship between frequency and pressure is basically linear. However, at about 3.8 GPa, the frequency–pressure slope of the Raman peaks of ascorbic acid changes significantly. The four linear equations at 562,

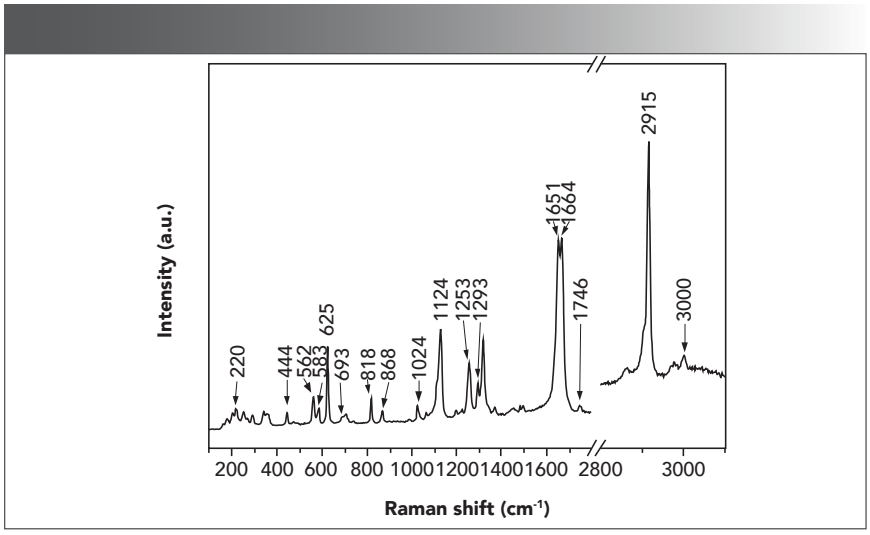

FIGURE 2: Raman spectrum of ascorbic acid at ambient conditions.

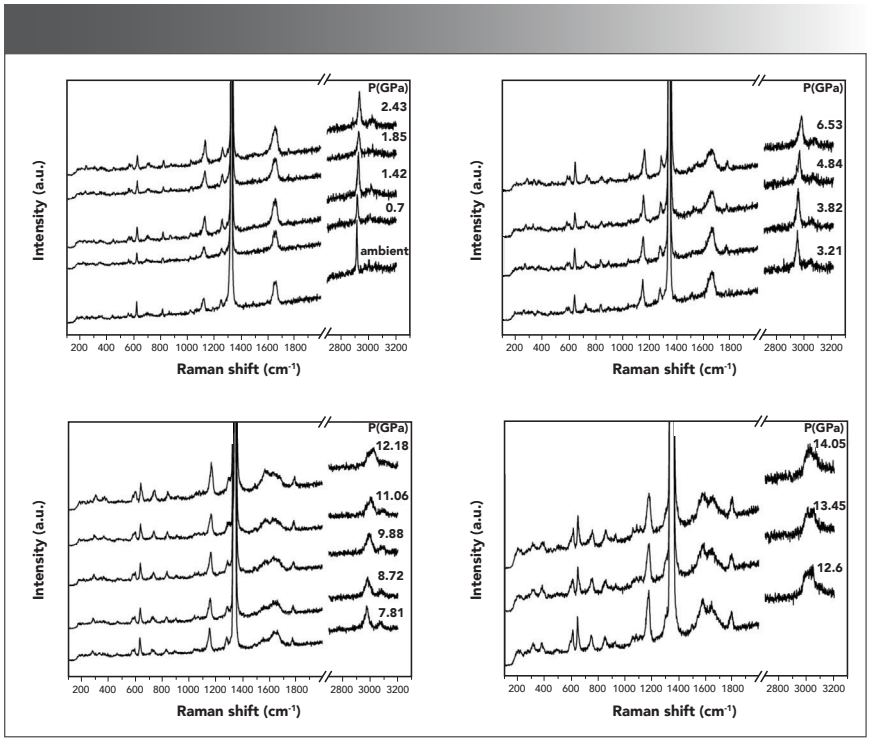

FIGURE 3: Selected high-pressure Raman spectra of ascorbic acid from ambient pressure to 14.05 GPa.

624, 693, and 3000 cm^{-1} are changed from y = 3.2708x+563.19, y = 2.377x+625.15, y = 7.3727x+695.54, and y = 9 .85x+3004.54 to y = 1.84702x+565.392, y = 1.3612x+626.75, y = 3.285x+700.8, and y = 6.545x+3022.8287, respectively (*x* represents pressure [GPa], and *y* represents Raman shift [cm^{-1}]). The sudden changes in the frequency-pressure relationship should correlate with the material phase transition. Therefore, we believe that a first-order phase transition of ascorbic acid occurs at approximately 3.8 GPa. We define the phase under pressure of 3.8 GPa as phase I, and when the pressure is higher than 3.8 GPa as phase II. The change in the molecular properties of ascorbic acid caused by phase transition remains a subject to be studied.

Additionally, a change in the symmetry of the molecular point group in ascorbic acid appears to accompany the phase change at 3.8 GPa. New bands at 1510 and 1767 cm^{-1} appear in phase II, indicating that the symmetry of ascorbic acid in phase II is lower than phase I. This also may be related to the fracture and rearrangement of the H-bond structure. Due to the effect of high pressure, most of the frequency–pressure Raman peaks of ascorbic acid become smaller. We also believe that the bonds in the crystal become more rigid after the phase transition.

Conclusion

In this work, we used high–pressure Raman spectroscopy (~14 GPa) to study the structure and Raman spectra of ascorbic acid. By observing changes in peak positions and intensities at approximately 583, 693, and 1746 cm^{-1}, it is shown that the internal and side chains of the ascorbic acid ring are changed under high pressure. Furthermore, we analyzed the frequency–pressure relationship of ascorbic acid, and found that ascorbic acid undergoes a phase transition at 3.8 GPa, and the symmetry of the crystal structure also changes. We hope that the results of this study can provide some insights into the study of the structure of ascorbic acid under high pressure.

Acknowledgments

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References

(1) R.W. Berg, *Appl. Spectrosc. Rev.* **50**(3), 193–239 (2015).

(2) B.M. Tolbert, M. Downing, R.W. Carlson, et al., *Ann. N. Y. Acad. Sci.* **258**(1), 48–69 (1975).

(3) W. Haijia, *Study on the Stability of Vitamin C and the Determination of the Content of Fruits, Vegetables and Fruit Juice by Ultraviolet Spectrophotometry,* Shanxi Medical University (2015).

(4) E. Cadenas and Lester Packer, Eds. *Handbook of Antioxidants, Vol. 712* (Marcel Dekker, New York, New York, 2002).

(5) C.Y. Panicker, H.T. Varghese, and D.

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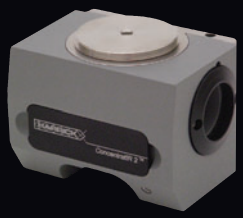

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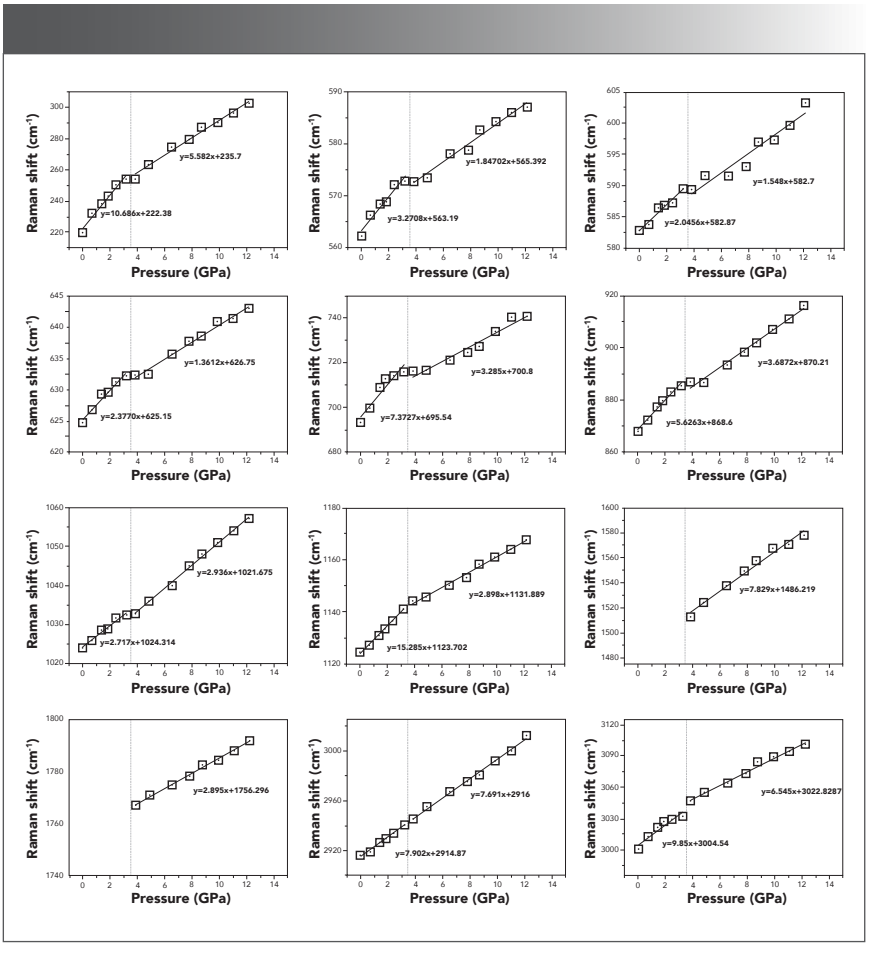

FIGURE 4: The frequency–pressure relationship of ascorbic acid.

Philip, *Spectrochim. Acta, Part A* **65**(3–4), 802–804 (2006).

(6) L. Packer, *Vitamin C in Health and Disease* (Marcel Dekker, New York, New York, 1997).

(7) O. Arrigoni and M.C. De Tullio, *Biochim. Biophys. Acta, Gen. Subj.* **1569**(1–3), 1–9 (2002).

(8) G. Singh, B.P. Mohanty, and G.S.S. Saini, *Spectrochim. Acta, Part A* **155,** 61–74 (2016).

(9) I.M. Lee, *Proc. Assoc. Am. Physicians* **111**(1), 10–15 (1999).

(10) A.C. Carr and B. Frei, *J. Am. Coll. Nutr.* **69**(6), 1086–1107 (1999).

(11) R.E. Patterson , E. White, A.R. Kristal, et al., *Cancer, Causes Control, Pap. Symp.* **8**(5), 786–802 (1997).

(12) K.A. Head, *Altern. Med. Rev.* **3**(3), 174–186 (1998).

(13) K.N. Prasad, A. Kumar, V. Kochupillai V, et al., *J. Am. Coll. Nutr.* **18**(1), 13–25 (1999).

(14) L. Beer, J.L. Brusso, R.C. Haddon, et al., *J. Am. Chem. Soc.* **127**(51), 18159–18170 (2005).

(15) K.W. Chapman, G.J. Halder and P.J. Chupas, *J. Am. Chem. Soc.* **131**(48), 17546–17547 (2009).

(16) F.J. Lamelas, Z.A. Dreger, and Y.M. Gupta, *J. Phys. Chem. B* **109**(16), 8206–8215 (2005).

(17) A. Olejniczak, K. Ostrowska, and A. Katrusiak, *J. Phys. Chem. C* **113**(35), 15761–15767 (2009).

(18) I. Hernandez and W.P. Gillin, *J. Phys. Chem. B* **113**(43), 14079–14086 (2009).

(19) R.O. Goncalves, P.T.C. Freire, H.N. Bordallo H N, et al., *J. Raman Spectrosc.* **40**(8), 958–963 (2009).

(20) M. Zhou, Z. Li, Z. Men, et al.,*J. Phys. Chem. B* **116**(8), 2414–2419 (2012).

(21) L. Sun, Y. Zhao, Y. Shang, et al., *Chem. Phys. Lett.* 689, 56–61 (2017).

(22) S. Meijiao, W. Kai, X. Shengnan, et al., *Spectroscopy and Spectral Analysis* **34**(5), 1302–1305 (2014).

(23) Z. Ma Z, J. Li, C. Liu, et al., *Sci. Rep.* **7**(1), 4677 (2017).

(24) P.F. McMillan, in *High-Pressure Crystallography,* A. Katrusiak and P.F. McMillan, Eds. (Kluwer, Dodrecht, The Netherlands, 2004), pp. 367–392.

(25) V.L. Solozhenko, in *High-Pressure Crystallography,* A. Katrusiak and P.F. McMillan, Eds. (Kluwer, Dodrecht, The Netherlands, 2004), pp. 411–428.

(26) P.F. McMillan, *Nat. Mater.* **1**(1), 19 (2002).

(27) W.L. Liu, Z.R. Zheng, R.B. Zhu, et al., *J. Phys. Chem. A* **111**(40), 10044–10049 (2007).

(28) C. Sun, H. Zhao, C. Liu, et al., *J. Raman Spectrosc.* **48**(8), 1127–1131 (2017).

(29) V.V. Mozhaev, K. Heremans, J. Frank, et al., *Proteins: Struct., Funct., Bioinf.* **24**(1), 81–91 (1996).

(30) R.J.C. Lima, A.M.R. Teixeira, P.T.C. Freire, et al., *J. Raman Spectrosc.* **32**(1), 27–32 (2001).

(31) H.K. Mao, P.M. Bell, J.W.Shaner, et al., *J. Appl. Phys.* **49**(6), 3276–3283 (1978).

(32) J. Hvoslef, *Acta Crystallogr., Sect. B: Struct. Crystallogr. Cryst. Chem.* **24**(1), 23–35 (1968).

(33) J. Hvoslef, *Acta Crystallogr., Sect. B: Struct. Crystallogr. Cryst. Chem.* **24**(11), 1431–1440 (1968).

(34) C. Mitterdorfer, J. Bernard, F. Klauser, et al., *J. Raman Spectrosc.* **43**(1), 108-115 (2012).

(35) Q. Li, S. Li, K. Wang, et al., *J. Chem. Phys.* **138**(21), 214505 (2013).

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2020 Review of New Spectroscopic Instrumentation

Howard Mark and Michael S. Bradley

We present our annual review of products introduced at Pittcon or during the previous year, broken down by the following categories: accessories, atomic spectroscopy, components, imaging, mass spectrometry, mid-infrared (mid-IR) spectroscopy, near-infrared (NIR) spectroscopy, nuclear magnetic resonance (NMR), Raman spectroscopy, software, ultraviolet-visible (UV-vis) spectroscopy, and X-ray.

This review focuses on new instrumentation, components, and accessories launched from May 2019 through April 2020, announced either directly to *Spectroscopy* through form submissions or by those presented as new at the recent Pittsburgh Conference (Pittcon) in Chicago, Illinois, where we spoke directly with vendors.

This year's Pittcon was interrupted by a larger societal concern—the sudden spread of the coronavirus. Pittcon was not canceled, but many exhibitors chose not to attend. Even so, there were still a large number of exhibitors, representing a cross section of the industry (from smaller suppliers to large instrument companies). The total attendance, reported as 9011, was, nevertheless, quite respectable, despite the challenges.

In this review, we are interested only in products that fall under the umbrella of spectroscopy, whether they be instruments, components, accessories, standards, software, or anything else related to spectroscopic measurement.

Excellence Awards at Pittcon 2020

One of the points of interest at Pittcon is the awards for instruments considered the most innovative. This evaluation is, of necessity, subjective, and involves a selection from among all the instruments on display at Pittcon. Starting three years ago, the selection methods and criteria were changed, and the awards are now called the Pittcon Total Excellence Awards. A selection committee, consisting of a blue-ribbon panel of experts, evaluates the entries based on ingenuity, creativity, implementation, and outcomes. Instruments are categorized by the size of the company (small, medium, and large) that makes them, based on their sales figures. This allows companies to compete with others in their same class. There are gold, silver, and bronze awards in each category, for a total of nine awards. We are pleased that this year four awards went to spectroscopy instruments. In the small company category, Waveguide won the gold for world's first small, battery-powered, handheld NMR instrument and Aeris Technologies won bronze for a real-time mid-IR-based ultrasensitive ethylene oxide gas analyzer. In the large-company category, Bruker won gold for its Lumos 2 FT-IR microscope, and Horiba won bronze for the LabRam Soleil instrument that combines Raman, UV-vis, and NIR spectroscopy.

The review that follows is organized alphabetically by wavelength

TABLE I: Index of companies and the categories where their products appear

Company Name	Category Listed Under
Agilent Technologies	Raman
Alliance Corporation	Accessories
Andor Technology	Imaging
Armadillo Sia	Components
Art Photonics	Accessories
Avantes, Inc.	NIR
B&WTek, a Metrohm Group Company	Raman
Bossart Analytics	Software
Brightspec, Inc.	Mid-IR
Cobolt, a part of Hübner Photonics	Components
Coherent, Inc.	Accessories
Dino-Lite Scopes	Imaging
Eblana Photonics Ltd.	Components
Edax Inc	Imaging
Edinburgh Instruments	Raman, UV-vis
Eigenvector Research	Software
Electro-Optics Technology	Components
Elementar Analysensysteme GmbH	Mass spectrometry
Elvatech Ltd.	X-ray
EssentOptics Ltd.	Mid-IR, NIR, UV-vis
Excellims Corporation	Mass spectrometry
Galaxy Scientific, Inc.	NIR, Accessories
Hiden Analytical	Mass spectrometry
Horiba Scientific	Raman, UV-vis and NIR
HySpex by NEO	Imaging
Ionicon Analytik	Mass spectrometry
IXRF Systems	X-ray
JEOL USA, Inc.	Mass spectrometry
Kaiser Optical Systems	Raman
McPherson	UV-vis
Metrohm USA	Raman
MKS Spectra-Physics	Components
Nireos	Imaging
Ocean Insight	NIR, Raman, UV-vis, Software, Components
Olympus Corporation of the Americas	Imaging
OPCO Laboratory, Inc.	Components
Photonis Scientific, Inc.	Imaging
Princeton Infrared Technologies, Inc.	Imaging
PS Analytical	Atomic
Reflex Analytical Corporation	Mid-IR, Accessories

Continued on Page 30

region or type of spectroscopy—for example, mid-infrared (IR), Raman, X-ray, and so forth—except that we place the two non-instrument categories (accessories and components) at the end. Table I sorts the companies alphabetically, and lists the categories they appear in. We arrange our review to allow readers to compare instruments from different manufacturers, although this process sometimes classifies low-end handheld instruments with high-end research tools. The categories used to classify the products are:

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

Our categories fluctuate from year to year, depending on trends in the submissions. The core spectroscopy headings are consistent, but the imaging category, for example, has been transient. This year, we received enough products classified as imaging to warrant that being a category in itself, rather than only including imaging versions of various technologies under the parent instrument type. Fluorescence was a popular category some time ago, but has fallen out of favor for several years. Last year it returned, but that proved to be only temporary; this year, there were again no submissions in that category, despite its analytical popularity and presence at trade shows.

As in the past, *accessories* are tools used with an instrument—like sample preparation or optical devices—whereas *components* are parts used as integral parts within

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Continued from Page 28

TABLE I: Index of companies and the categories where their products appear (continued)

Company Name	Category
Savillex	Accessories
Shimadzu Scientific Instruments	UV-vis
Sierra-Olympic Technologies, Inc.	Imaging
Si-Ware Systems	NIR
SouthNest Technology Co., Ltd.	NIR
Spectral Evolution	Accessories, NIR
Spectrolight	Components
Spetec GmbH	Accessories
S.T. Japan-Europe GmbH	Software
ST Raman 1064	Raman
Thermo Fisher Scientific	Atomic, Raman, Software
Tornado Spectral Systems	Software, Accessories
UniKLasers Ltd	Components
Unity Scientific	Software
Wasatch Photonics	NIR, Raman, Accessories
Waveguide	NMR
WITec GmbH	Raman

instruments, like lasers or detectors. The software category includes instrument control and data processing, storage, and transmission, as well as spectral databases (libraries) and other collections of specialized information, besides programs that analyze the data.

Overview: Trends

One of our goals in writing this instrumentation review, as well as spending time at instrumentation trade shows (such as Pittcon), is to identify larger themes from the aggregation of submissions.

Some years ago, we had seen environmental solutions trending, especially around microplastics. This year, environmental issues were muted under the public health solutions around opioids, cannabis, and COVID-19. The plenary lecture at Pittcon, and many hallway conversations, were dominated by these subjects, and vendors were touting testing and research tools. The absence of several vendors, especially from Asia and some parts of Europe (and the reticence of attendees to shake hands), put an exclamation point on this.

Within the instrument submissions themselves, we see many tools and instruments relating to Raman spectroscopy. We discuss this further in the Raman spectroscopy section, but note here that component and accessory suppliers, as well as instrument manufacturers, have identified Raman spectroscopy as a significant market. Overall, we saw in recent years many handheld instruments and new laser sets, and also found that large instruments and software were prevalent this year.

In the expanding world of software, we reported last year on the emerging uses of computers in artificial intelligence (AI) applications and integrating with the internet of things (IoT), as expansion of IoT is starting to come to fruition, albeit not as soon as we originally expected. We note this in our review below.

One continuing trend was the combination of various technologies into a single instrument. Several companies, for example, are now combining Raman spectroscopy with other optical spectroscopies, such as UV-vis or infrared. These combinations are often augmented with special software to enable the instrument control computer to find commonalities or other relationships between the spectra produced by the different technologies. Some details about this are apparent in the Raman spectroscopy section of this review.

Vendors have all identified the trend in many laboratories of downsizing staffing, even with a continued increase in sample loads. This means a single worker must be able to move between multiple instruments without major barriers. Easy sample transfer and shallow learning curves via workflow software are becoming common needs. With instrument vendors, this information is often buried, both in their product development and their marketing literature, under the prevalent and long-standing emphasis on hardware performance (signal-to-noise, resolution, speed, and so forth), but it becomes immediately apparent when you watch vendors demonstrate their instruments. The demonstration is increasingly a software show. This trend is discussed further in the software section of this review.

This year, we added a new tactic for the trend predictions. We contacted subject-matter experts to discuss future trends in their technologies. We thought that people working in the same area might be seeing the same forces affecting their technology. Below, we share some of the responses we received to this inquiry. Because these comments represent opinions rather than hard facts, to preserve privacy, we do not identify the company or person responding with each com-

TABLE II: Atomic spectroscopy products

Company Name	Product Name	Product Type	Measurement Mode	Applications, Features, and Benefits
PS Analytical	Online Hg Waste Water Analyzer 10.226	Mercury analyzer	Atomic fluorescence	An automated self-calibrating unit offering ultralow reagent use (<5 mL per test) and ultralow detection capability (sub ppb). Multiple alarm options with several sample streams available. No longer requires continuous flow of reagents. A discrete approach is used. An option for any industry that requires monitoring of Hg in wastewater (coal-fired power industry, petrochemical produced water, municipal installations, semiconductor industry).
	Mercury Workroom Air Monitor 10.216	Mercury analyzer	Atomic fluorescence	An automated self-calibrating unit offering continuous Hg monitoring for 24/7 protection. Multiple alarm options with multiple sample streams are available. An option for any industry that uses or processes Hg (reprocessing of petrochemical catalysts, fluorescent tube manufacture, battery manufacture, chloralkali industry, semiconductor industry).
Thermo Fisher Scientific	iCAP Pro Series	ICP-OES	ICP-OES	This platform provides a fast, sensitive range of trace element analysis solutions using inductively coupled plasma–optical emission spectroscopy (ICP-OES). Through the use of a single optical slit and a charge injection device detector, the new instruments reduce the number of measurements per run needed to capture a complete spectrum, increasing speed of analysis and readout. With a start-up time of only 5 min, the platform also maximizes instrument uptime, enhances workflow productivity, and reduces cost-per-sample and minimizes recalibration requirements.

TABLE III: Imaging products

Company Name	Product Name	Product Type	Measurement Mode	Applications, Features, and Benefits
Andor Technology	Balor-X	sCMOS camera	Indirect detection	Unlike other cameras, Balor-X combines a large 16.9 megapixel sensor with the fast readout speed of sCMOS technology, giving 54 FPS at full frame. This is complemented by the high sensitivity and low readout noise of sCMOS technology. The only camera on the scientific camera market to combine such a large field of view, frame rate, and sensitivity. Applications include X-ray and neutron in situ experiments. A large field of view and fast frame rates enables this camera to capture transient dynamic phenomena at high resolutions and speeds. It is versatile, and can be used for both large sample radiography and smaller samples at high resolution.
Dino-Lite Scopes	Dino-Lite	Imaging microscope	N/A	This product provides high-quality microscopy video interfacing to a PC or Mac. Most models provide 10–220x magnification. Options include measurement, adjustable polarizer, and software that makes it easy to take snapshots, record videos, manipulate images, and save and email discoveries.
Edax Inc.	Velocity Series EBSD camera series	N/A	N/A	The Velocity Camera Series offers high-speed EBSD mapping with the best indexing performance on real world materials. Powered by a CMOS sensor, the Velocity combines fast acquisition with high-sensitivity and low-noise performance. The performance of the cameras extends to a wide range of materials, including lower symmetry, multi-phase and deformed structures. This camera is available in two models: the Velocity Plus (up to 3000 indexed points per second) and the Velocity Super (up to 4500 indexed points per second). For both models, these speeds can be achieved while providing indexing success rates up to 99% or better. Applications include lower symmetry, multi-phase, deformed structures, in-situ EBSD, 3D EBSD, scanning electron microscopes (SEMs), electron backscatter diffraction (EBSD).
HySpex by NEO	Baldur	Hyperspectral imagers (HSI)	N/A	Baldur industrial hyperspectral imagers are fast, flexible, robust, and repeatable, with spectral resolution of two bands, capturing 4x more light as Hyspex's classic systems. Baldur imagers can be configured from 400 to 2500 nm with multiple independent regions of interest and measurement length range. HySpex offers seamless integration of HW and Prediktera data processing software, with excellent capability to collect high quality data, while creating and transferring actionable information to downstream devices.
Nireos	Hera	Hyperspectral camera	N/A	Imaging using the Fourier-transform approach results in very high sensitivity because of much higher throughput than dispersive cameras, and exceptional spectral resolution at 400 nm wavelength (< 1 nm). The camera captures images in a static regime. Hera is the first hyperspectral camera from Nireos. The camera offers low-light applications, and applications where moving the camera or the sample is difficult. Common applications are fluorescence imaging, cultural heritage, molecular biology, astronomy, agriculture, food quality, mineralogy, and geology.
Olympus Corporation of the Americas	DSX1000	Digital microscope	N/A	Guaranteed high- and low-magnification accuracy and precision using a single instrument, with 20–7000x magnification range. Fully motorized optical zoom eliminates common manual errors· Quick-change objective lenses enable completing inspections faster. Spot hard-to-see defects with a flexible tilting head and rotating stage. Switch between six observation methods with a single click.
Photonis Scientific, Inc.	Mantis3	Single-photon counting camera	N/A	A single-photon-counting camera with nanosecond time-stamping, and <10 μm spatial resolution. Mantis3 consists of a Timepix3-based visible light camera coupled to Cricket, containing a high-end image intensifier. The TPX3Cam is a high-rate, event-driven, time-stamping camera. The Cricket enables single-photon sensitivity, and offers a choice of photo-cathodes optimized for your application. The TPX3Cam is offered in collaboration with Amsterdam Scientific Instruments.

TABLE III: Imaging products (continued)

Company Name	Product Name	Product Type	Measurement Mode	Applications, Features, and Benefits
Princeton Infrared Technologies, Inc.	SWIR Mega-pixel MVCam	SWIR megapixel MVCam	Reflection and emission	The compact SWIR–visible camera supports the highest commercially available frame rate at megapixel resolution with no ITAR restrictions. High resolution (1280 x 1024 pixels) SWIR imagery at up to 95 frames/s. Advanced digital array (PIRT1280A1-12) detector generates 14-bit image data, and read noise less than 45 e-, This camera does not have deep cooling, allowing it to be 11x smaller in volume, use 6x less power, and is 84% lighter.
Sierra-Olympic Technologies, Inc.	Ventus Compact	Mid-IR imaging	N/A	The Ventus Compact combines the functionality of earlier Ventus systems with an integratable package, making it the smallest, lightest, most power-efficient camera in the Ventus product line. The Ventus Compact features continuous zoom, one-touch autofocus, advanced image processing, and a unified easy-to-integrate software architecture. It is equipped with advanced "NUC Through Zoom" calibration and a compact low-SWaP package.

ment, but we list the expected trends for the technology. For those companies that responded to this question and have multiple products, their response is listed under the technology category that their instrument containing the response belongs.

Imaging

- "[There is] a general trend towards higher resolution X-ray and neutron indirect detection cameras."
- "[There is a] continuous trend of improving the data storage, handling, and processing allowed hyperspectral imaging to take place as it generates very heavy images. One image captured by [tradename redacted] can require 1 Gb [of data], as it contains a lot of information of a scene."
- "Shortwave infrared (SWIR) imaging is growing in many biological and chemical analysis applications."

TABLE IV: Mass Spectrometry products

Company Name	Product Name	Product Type	Measurement Mode	Applications, Features, and Benefits
Elementar Analysensysteme GmbH	BiovisION Honey	Mass spectrometry	Carbon isotope ratios	High temperature oxidation for the detection of C3 sugar adulteration of honey via carbon isotope analysis. The system is simpler to use, significantly more robust, and has reduced running costs compared to traditional techniques, increasing the chances of detecting fraudulently adulterated honeys. This mass spectrometry (MS) method for detecting honey replaces wet chemical oxidation techniques. BiovisION Honey uses a completely new technique: high-temperature oxidation, followed by MS analysis to determine isotope ratios. This method offers higher throughput, simpler analysis, and better return on investment, ultimately making it cheaper to detect fraudulent honey adulteration.
Excellims Corporation	MC3100 Compact HPIMS-MS	Ion-mobility mass spectrometry	Ion mobility	This product combines Excellims' mobility technology (HPIM-STM) with a miniaturized ion trap mass spectrometer. This is the first small-footprint analytical system that identifies chemicals based on both ion mobility and *m/z*; it offers superior isomer separation and chemical identification capability, while providing chemical structure information via direct collision cross-section measurements. Combining library-based analysis in two dimensions and prefiltering capability, the MC3100 is ideal where speed, specificity, and fieldability are important.
	GA2200	Mass spectrometry with compact integrated autosampler	Ion mobility and mass spectrometry	A high resolving power (R > 70) ion mobility spectrometer optimized for use in cleaning validation. It provides API-specific analysis in 30–60 s, without the need for columns or a vacuum system. It offers electrospray ionization for a wide range of APIs and detergents in various solvents, straightforward method development, and analysis of new compounds. The product is 21 *CFR* part 11 compliant, and has a compact integrated autosampler, controlled by the GA2200's 21 *CFR* Part 11-compliant software.
Hiden Analytical	SIMS-ToF	Mass spectrometry	ToF secondary ion	The SIMS-ToF provides high surface sensitivity, wide mass range and parallel detection for both the SIMS Workstation range as well as being a crucial addition to other surface analysis instruments. The time-of-flight detector gives rapid identification of surface chemistry and distribution using 3D imaging format with upper monolayer specificity.
	pQA	Portable quadrupole analyzer	Quadrupole	The Hiden pQA portable gas analyzer is a versatile mass spectrometer and is offered with a range of interchangeable sampling inlets to suit a broad application range. MIMS inlets are offered for analysis of dissolved species in ground water, fermentation cultures, soil samples, and general applications where analysis of dissolved species in liquid sample is required.
	DLS-20 QMS	Ultrahigh resolution quadrupole mass spectrometry	Quadrupole	The Hiden DLS-20 QMS is a quadrupole mass spectrometer specifically designed for the analysis of hydrogen and helium Isotopes and light gases, and includes a new Hiden mass filter designed for ultra-high resolution. The new mass filter design is a micron precision assembly, using the finest precision machined components.
	HPR-40 DSA	Membrane inlet mass spectrometry (MIMS)	Differential electrochemical mass spectrometry (DEMS)	The Hiden HPR-40 DSA Membrane Inlet Mass Spectrometer (MIMS) is a compact benchtop gas analysis system for real-time quantitative analysis and monitoring of dissolved or evolved gases. The system is available with a range of differential electrochemistry mass spectrometry (DEMS) cells. DEMS cells include a nanoporous membrane interface for fast response for in-situ determination of gaseous and volatile electrochemical reactants, reaction intermediates, and products in real time.
	QGA	Quantitative gas analyzer		The Hiden QGA is configured for continuous analysis of gases and vapors at pressures near atmosphere. Can also be configured for the system for sampling from low to high pressures, up to 30bar. Suggested applications include high purity gas analysis, fermentation, fuel cells, gas production and storage, environmental monitoring, gas separation studies, near atmospheric XPS, and APXPS at pressures near atmosphere in standard form.

Mid-IR spectroscopy

- "Rapid growth of several industrial market segments (including chiral chemicals, asymmetric synthesis, cannabinoids, essential oils, and others) have created a strong demand for analytical techniques capable of fast isomer-selective chemical analysis. The emerging [trade-name redacted] technology addresses this demand, ... offer[ing] extraordinary chemi-

TABLE IV: Mass spectrometry products (continued)

Company Name	Product Name	Product Type	Measurement Mode	Applications, Features, and Benefits
Ionicon Analytik	Charon	PTR-TOF Mass spectrometer	TOF	An all-in-one monitoring for trace gas & organic particles. Versatile, reliable, and proven technology for VOC analysis. Characterize a wide range of organic compounds in the gas- and particle-phase with a single instrument. Direct analysis of the VOC, IVOC, SVOC, and LVOC range as well as particles. Applications: Environmental research, engine exhaust analysis (including diesel), exhaust from aircraft and cars, electronic nicotine delivery system (ENDS).
	PTR-TOF 1000 X2	TOF Mass Spec	TOF hexapole ion guide	The PTR-TOF 1000 X2 is the base instrument with an X2 option, a combination of the Ion-Booster and the hexapole Ion-Guide. This increases the sensitivity beyond previous limits. The instrument comes with 10,000–20,000 cps/ppbv, delivering low detection limits with short integration times, due to new and improved hardware components. The X2 increases instrument sensitivity 10x and sets a new benchmark in PTR-MS. Suggested applications include measurement of extremely low concentrations of VOC samples in research such as forests, isolated or rural areas, and airborne flight research campaigns. Another application is monitoring airborne molecular contamination in cleanrooms where contamination levels are already very low.
JEOL USA, Inc.	Spiral-TOF	Imaging MALDI-TOF/ TOF Mass Spectrometer	N/A	This matrix-assisted laser desorption ionization (MALDI) mass spectrometer system offers ultrahigh mass-resolving power and optional MS/MS with unit-mass precursor selection for imaging samples that are not perfectly flat. Imaging speed is increased by a factor of up to 5 by optimizing sample irradiation and stage motion.

TABLE V: Mid-IR products

Company Name	Product Name	Product Type	Measurement Mode	Applications, Features, and Benefits
Brightspec Inc.	IsoMRR	Far-IR spectrometer	Molecular rotational resonance spectrometer	A spectrometer that measures rotational spectra to identify species based on differences in their 3-dimensional mass distributions, isoMRR brings a much higher level of selectivity to isomer and isotope analysis than MS. Benefits include abilities to ID and quantify all types of isomers and isotopologues directly in crude mixtures, and perform chiral and achiral analyses for chemically diverse analytes in one measurement. Brightspec reports that isoMRR is the only spectrometer of this type available on market.
EssentOptics Ltd	Photon RT spectro-photometer for coaters	Mid-iR, NIR, and UV-visible spectrometer	Transmission and absolute reflection measurements at variable AOI's and polarizations	This instrument is specifically designed to measure optical coatings. It has the widest wavelength range, 185–5200 nm, in a single instrument. Transmission and absolute reflection measurements at variable AOIs and polarizations. Transmission measurement of thick samples or complex cemented prisms, with beam off-set up to 60 mm. The configuration with 185–5200 nm wavelength range is brand new, and more powerful and advanced than previous versions. New features include also a new gratings turret, upgraded monochromator, an auto-detect stage-base for motorized stages, and more.
Reflex Analytical Corporation	FAME	Biofuel analyzer	N/A	Samples measures the fatty acid methyl ester (FAME) content of biodiesel fuels, down to concentrations of 0.02%, using ASTM methods using FT-IR spectroscopy. Analysis time is <1 min for each sample. Combined with an autosampler, fully automated measurement of even larger sample numbers is possible.

cal specificity combined with fast analysis and ease of use."
- "Photonics devices [will] become much more advanced. This requires [technicians] to use optical components with extreme specifications. These specifications need to be measured and confirmed, so this leads to design of more advanced metrology and testing equipment."

NMR

- "Close to 20 years ago, the first portable X-ray fluorescence (XRF) devices were released for easy-to-use metal and mining applications for non-scientific users. A decade ago, there was a strong thrust into the portable optical/vibrational spectroscopy market, with Raman, NIR, and FT-IR for safety, security, military, and pharmaceutical raw-material ID analysis. One company [name redacted] extends this portable theme further with the world's first portable NMR, which addresses the gaps of XRF and optical and vibrational [spectroscopy] in the areas of biologics, vaccines, foods, and, ultimately, in medical diagnostics. The theme or trend is routine chemical screening and non-scientific operators who need to make a fast and precise decision at the point of need."

Raman spectroscopy

- "The pharmaceutical industry is not making large investments at this time, as market consolidation and acquisitions are on the rise in this sector. The demand for field identification of controlled substances and threats is global, with needs specific to geographic regions. Investment in technology is tied to national budgets, and therefore impacted by geopolitical and global economic trends."
- "With continued improvements in Raman technology, more sophisticated trace-level and low-concentration measurements are becoming possible."
- "Automation is among the most important long-term trends in the development of scientific instruments. Using optimization and calibration routines, along with pre-set and saved experimental workflows, reduces input demands on the researcher, while allowing them to focus on the data they acquire. Errors are minimized, while operational turnover is maximized, enabling laboratories and user facilities to generate more, and more consistent, data within a given amount of time."
- "I am seeing increasing interest in cloud-based analytical solutions—instrument management and reporting, mostly—from both customers and multiple vendors."

Software

- "Hyperspectral imaging is [a] growing field that is finding applications in processing, medical imaging, environmental applications, and earth sensing. [Trade-name redacted] allows incorporation of domain knowledge necessary for interpretable results required by engineers and scientists."
- "Chemometrics is falling under a broader field of data science and machine learning. In addition to AI tools, our package is more flexible than most tools, and allows incorporation of domain knowledge necessary for interpretable results required by engineers and scientists."

TABLE VI: NIR products

Company Name	Product Name	Product Type	Measurement Mode	Applications, Features, and Benefits
Avantes, Inc.	AvaSpec-MiniNIR	Miniature NIR spectrometer	Raw data, transmission, reflection, absorbance, absolute and relative irradiance	A small form factor, high resolution, high sensitivity uncooled InGaAs spectrometer. Easy to integrate into other devices, including OEM handheld applications. Well suited for various applications, including food analysis, security monitoring, and the recycling industry.
Essent Optics Ltd	Photon RT spectrophotometer for coaters	UV, visible, NIR, and mid-IR	Transmission and absolute reflection	Please see the Mid-IR table for the product details.
Galaxy Scientific Inc.	NF2000	FT-NIR with fiber optic probe	Reflectance or transmission	Compact, portable, and high-performance FT-NIR spectrometer with triggered fiber optic probe for laboratory and field, Built-in probe holder. Designed from the ground up to offer a new kind of NIR analysis solution. Brings together the portability required to move NIR analysis closer to point-of-need, combined with excellent spectroscopic performance for the fastest and most accurate results.
Ocean Insight	Ocean HDX-XR	UV-vis-NIR spectrometer	Absorbance, transmission; irradiance; color; reflectance	Please see the UV-vis table for the product details.
	Nano-Quest	NIR Spectral Sensor	Absorbance, transmission, reflection	Ocean Insight has launched a compact spectral sensor for qualification and quantification of materials from 1350 to 2500 nm (7400–4000 cm^{-1}). NanoQuest is a MEMS-based FT-NIR spectrometer that provides extended spectral range and exceptional performance in a package that is considerably smaller and more accessible than traditional lab-based instrumentation.
Si-Ware Systems	NeoSpectra-Scanner	Portable and handheld spectral sensing device	Reflectance	The scanner is a hardware- and software-ready device that enables field material analysis applications. The scanner operates over a wide spectral range in the NIR, offering optimum results. The scanner has a large spot size for measurement of heterogeneous samples, a rugged ergonomic design (IP65), is battery operated, is Bluetooth compatible, and incorporates the NeoSpectra-Micro sensor, a Fourier-transform IR (FT-IR) technology that offers a wide spectral range (1350–2500 nm). It uses the same technology as the NeoSpectra-Micro, with a market-ready solution for resellers that can take months or years off unique application development.
SouthNest Technology Co., Ltd.	NanoFTIR NIR spectrometer	FT-NIR and FT-IR spectrometer	Transmission, reflection	An FT-IR and FT-NIR system based on MEMS technology. The larger FT-IR mirror size (mm range) allows more light to enter the system, improving signal quality. The wavelength covers almost the whole NIR range from 900 to 2500 nm. The spectrometer has good anti-vibration performance. Applications include smart farming (soil analysis, crop analysis, hay analysis), food process, and raw materials.
Spectral Evolution	OreXpert	Field NIR spectrometer	Transmission, reflectance, absorbance	This product offers the highest resolution available for harsh field use. High resolution for distinction of features help identify trace minerals. Covers the UV-vis-NIR range from 350 to 2500 nm, and features ultrahigh resolution and very stable performance, with three high density thermoelectrically cooled photodiode arrays. FWHM is: 1.5 nm @ 700 nm; 3.0 nm @ 1500 nm; 3.8 nm @ 2100 nm. The product is designed for mineral identification and analysis where there is a need to distinguish between minerals with similar spectra, or to more accurately identify mineral pathfinders.
	OreXplorer	Field-rugged NIR spectrometer	Transmission, reflectance, absorbance	Designed for field work with a rugged chassis, with no moving optical parts, and a field-replaceable rugged metal clad fiber optic cable. Features one-touch operation, with auto-dark current and auto-exposure. Communications include wireless Bluetooth and USB connection. It includes DARWin SP Data Acquisition software that is Windows 7/8/10 compatible. The oreXplorer provides high resolution and high sensitivity in a portable spectrometer for field or laboratory use.

TABLE VI: NIR products (continued)

Company Name	Product Name	Product Type	Measurement Mode	Applications, Features, and Benefits
Wasatch Photonics	WP NIR OEM spectrometer module	An off-the-shelf drop-in spectrometer designed for rapid OEM integration	Absorbance, transmission, reflection	This product covers a spectral range of 900–1700 nm, and is designed to deliver high signal-to-noise ratios at shorter acquisition times than traditional InGaAs-based diode-array spectrometers. The instrument integrates a VPH grating into a compact, robust optical bench, configured with an f/1.3 input for signal collection, and a TEC cooled detector. Custom designs are available upon request.
	WP VIS NIR OEM spectrometer module	Same as WP-NIR-OEM	Absorbance, transmission, reflection	Same as WP-NIR-OEM, except that the wavelength range is 350–1000 nm

TABLE VII: NMR products

Company Name	Product Name	Product Type	Measurement Mode	Applications, Features, and Benefits
WaveGuide Corporation	Wave-Guide formμla portable μNMR	Battery-powered, handheld NMR	Time domain NMR (21 MHz, 0.5 Tesla)	The world's first portable, battery-operated, NMR analytical instrument, optimized for scientific non-experts to make decisions in the field or the point-of-care. Applications include authentication of vaccines and biologics, anti-counterfeit, expired, or substandard medicine, foods, petrochemical, and medical diagnostics (tuberculosis screening) and a fast, low-cost, accurate method for the earlier detection of ovarian and other cancers. This instrument incorporates a breakthrough developed at Harvard University that enabled the miniaturization of NMR by a factor of more than 100x. WaveGuide's NMR operates within minutes between wide ambient and sample temperatures, and only requires ~30 μL of sample.

- "The increasing development of handheld or smaller sized spectrometers."
- "NIR in general is moving away from technology experts with years of training and experience, to users of the technology that need to get results. [Company name redacted] is responding by creating intuitive products that provide top performance and capabilities in a user-friendly format."
- "[Increasing use of the] home office."

UV-vis spectroscopy

- "General optimism and more government money being spent in science, especially [in the fields of] astrophysics and physics. For example, more of our customers are getting funded via National Science Foundation/Department of Energy, and even NASA."

Components

- "[Technology] is driving toward ever-lower scatter, while demanding high efficiency."

Accessories

- "Today's trace metals analysis laboratories are constantly being driven to achieve lower levels of detection, which, in turn, put greater demand on clean chemistry techniques and applications."
- "Increasing automation in the laboratory has led to a demand for easy-to-operate pumping systems that do not require pressure to be set individually."

Some current (and even past) practices may become future trends, if and when they become more widespread and generalized. In the meanwhile, sporadic mentions of these practices appear in advertisements, in scientific literature, and even in this review. For example, some instrument manufacturers have created a capability of remotely controlling and collecting data from their own instruments (networking) for a long time. As we said last year, when that capability expands to include more than one type of instrument, then it would be fair to rename that localized networking as belonging to IoT, but not until then. Similarly, can the current capabilities of the application of chemometric analysis to instrument data, to perform quantitative and qualitative analysis, be called *AI*?

As we have noted almost since we first started trying to detect instrument trends, the trend toward hyphenated techniques has been coming along slowly, but surely, over the years. A recent twist on that concept, broadening the idea of applying multiple technologies to an analysis, is the packaging of dissimilar, and indeed sometimes even orthogonal, technologies in a single instrument package, without the two technologies necessarily interacting (as hyphenated methods do). We first noted this trend several years ago, but, even in last year's

TABLE VIII: Raman spectroscopy products

Company Name	Product Name	Product Type	Applications, Features, and Benefits
Agilent Technologies	Vaya	Raman raw material identity verification system	Vaya is a handheld spatially offset Raman spectroscopy (SORS) system for QC testing of pharma and biopharma raw materials through containers. Vaya works through transparent and non-transparent packaging materials, increasing raw material ID verification throughput without increasing costs, by reducing the need for sampling. By incorporating conventional Raman and SORS technology in a handheld unit for use at GMP-compliant pharmaceutical sites, Vaya brings true through-barrier analysis to the handheld Raman market. Applications include through-container pharma, biopharma, and nutraceutical raw material identity verification testing, and counterfeit detection.
B&W Tek, a Metrohm Group Company	TacticID-N Plus and TacticID-GP Plus	Raman	Compact Raman for rapid field identification of substances, with easy reporting, embedded camera, safety information, and flexibility for non-destructive measurement of solids, liquids, and gels, with minimal sample preparation and contact. Color-coded results with overlay option. Interchangeable accessories. New this year are faster analysis times, increased data storage, and tests in accordance with the *USP, EP,* and *JP*. Safety information can be displayed with results, by an embedded camera. TacticID-N Plus is for identification of controlled substances by police officers, has a closed system with a library of >1200 compounds of interest and ability to measure low-dose drugs with a SERS accessory. TacticID-GP Plus, with a library of >10,000 compounds and ability for user-created libraries, is designed for HazMat and first responder teams, and customs and border protection for rapid on-site identification of potential threats.
	STRam-1064	Raman scattering specialized for see-through measurements	This product collects Raman signals generated underneath diffusive top layers to identify material inside visually opaque barriers such as plastic bottles, paper bags (kraft paper), and fiber sacks. Comprised of a high-throughput spectrometer, specialized multi-reflection sampling optics, and advanced algorithms in a compact design, the STRam-1064 delivers rapid material identification capabilities through barrier layers and packaging with minimal fluorescence, expanding Raman identification capabilities while maintaining sample and package integrity. The product is an expansion of the STRaman technology to a 1064-nm laser excitation system, giving improved performance for measurement through barrier layers, without fluorescence interference.
Edinburgh Instruments	RM5 Raman Microscope	Raman scattering	The truly confocal design of the RM5 is unique to the market, and offers uncompromised spectral resolution, spatial resolution, and sensitivity. Truly confocal, with variable slit and a multiple-position adjustable pinhole for higher image definition, better fluorescence rejection, and application optimization. The RM5 builds on the expertise of robust and proven building blocks, combined with modern optical design considerations. It has a focus on function, precision, and speed.
Horiba Scientific	LabRam Soleil Raman Microscope	Raman microscopy, Raman scattering, UV-vis-NIR imaging	The LabRam Soleil multimodal Raman microscope has ultrafast Raman imaging (100 times faster imaging to speed up analyses), full automation (to save time). and intuitive software (Enriched LabSpec Automation). This is the first multimodal Raman microscope designed for UV-vis–NIR imaging for research or QC departments. It provides images of unmatched precision and very-high-resolution spectra.
Kaiser Optical Systems, Inc.	Raman Rxn2 Multichannel	Raman scattering	Kaiser's new embedded technology integrates the spectrometer control and data handling functions into a Kaiser Raman analyzer, without needing a separate computer with proprietary software. Kaiser's embedded technology ensures 24/7 reliability, provides an easy-to-follow touch-screen user interface, and exports raw data and diagnostics. Suggested applications include pharmaceutical, biopharmaceutical, chemical, polymers, and food and beverage.
Metrohm USA	Mira	Reflectance Raman	The Mira is a flexible, handheld Raman spectrometer. It features smart tips, and dedicated sampling accessories that make handheld Raman more reproducible. The new iUA enables guided workflows with instrument-prompted position settings of the iUA. Surface, bag, or bottle settings provide optimized signal collection, faster scans, and fewer missed identifications. The Mira DS can scan through opaque containers and identify the material inside. Mira Cal Mobile is a new app that brings the power of a smartphone to handheld Raman: Operates Mira from a distance, add geotags, pictures, notes and more. Applications include: raw material verification, unknown identification, spill response, hazardous materials, customs and border patrol inspections, counterfeit identification.

TABLE VIII: Raman products (continued)

Company Name	Product Name	Product Type	Applications, Features, and Benefits
Ocean Insight	QE Pro-Raman+ Spectrometer	Raman scattering	A high-sensitivity, 785-nm Raman spectrometer providing low limits of detection for trace level materials identification. It delivers faster, cleaner Raman signatures out to 3000 cm^{-1}, with 3x sensitivity improvement and thermoelectric cooling for great stability. This next-generation spectrometer uses gold-coated mirrors, a back-thinned FFT-CCD detector, and higher-performance, wider-range grating to detect weaker, more elusive Raman signatures.
Thermo Fisher Scientific	DXR3	Raman microscope	Easy-to-use Raman microscope with point-and-shoot and mapping capabilities, all-new automatic X-axis calibration, improved stability and reliability, improved stability and reliability, available. Suggested applications: microplastics analysis, advanced polymer research and development, pharmaceutical drug research and development, material science, and battery and energy storage.
	DXR3xi	Raman imaging microscope	Fast imaging with real-time data visualization and comprehensive on-demand alignment and calibration tools. Includes particle analysis workflow and tools for automated identification of microplastics and contaminants; new 3D visualization software for enhanced exploration of z-stack chemical images, and automatic X-axis calibration as seen in the DXR3.
	DXR3 SmartRaman	SmartRaman spectrometer	Dedicated to bulk sample analysis with research-grade performance. Multiple dedicated interchangeable sample holders, plus automatic X-axis calibration as seen in the DXR3.
Wasatch Photonics	WP 785 ER	Raman spectrometer	The WP 785 ER extended range Raman spectrometer is designed to provide high sensitivity, fast acquisition rates, and low limits of detection out to 3500 cm^{-1}. The company's volume phase gratings (VPH) are integrated into the optical bench, designed with an f/1.3 input for maximum signal collection. The WP 785 ER can be configured for various applications with a choice of fiber-coupled or free space sample coupling, spectral range, and detector cooling (ambient, regulated, or TEC cooled). The WP 785 ER provides access to chemical information found in the functional group region, out to 3500 cm^{-1}.
	WP 785, WP 830 Raman spectrometer with integrated laser	Raman spectrometer	These Raman spectrometers feature a fully integrated 350 mW multimode laser that is both powered and controlled through the spectrometer in a single, compact unit. Dual fiber optic connectors allow coupling of a Raman probe or other sampling accessories to the unit for maximum flexibility. The streamlined design of this duo economizes on space and hardware cost, and allow the creation of reconfigurable, semi-integrated Raman systems.
WITec GmbH	alpha300 apyron	Confocal Raman imaging microscope	The new alpha300 apyron is an automated confocal Raman imaging system. Through software-driven control, the laser wavelength and output power, fiber coupling and beam alignment, focus, polarization, objective and spectrometer configuration can be selected to match the demands of each sample. These properties are automatically saved with the measurement for advanced Raman microscopy with a new level of reproducibility and ease of use. The system is especially well suited for multi-user laboratories with researchers of varying levels of experience with Raman microscopy and industry laboratories concerned with evolving experimental challenges and time-critical analysis. Suggested applications areas include working in materials science, environmental science, microparticle analysis, life science, food science, geology, pharmaceutics, and many others.

review, there was only one example of this combining of technologies, With hindsight, we can see the beginnings of this trend several years ago, when Raman spectroscopy was combined with an atomic force microscope (AFM) in one unit. In this review, there are multiple companies demonstrating combined technologies; interestingly, all of them include Raman spectroscopy as one of the technologies.

Some other potential miscellaneous trends can be seen if you keep your eye tuned for them, one of them being a change in the nature of applications from being chemistry-focused to becoming more focused toward biochemical and biomedical applications.

Review of New Products for 2020

Atomic Spectroscopy

Both Thermo Fisher Scientific and Perkin Elmer introduced new inductively coupled plasma (ICP) solutions, striving for increased sensitivity and speed. In presenting these instruments, these companies focus on use in a wide range of markets

TABLE IX: Software products

Company Name	Product Name	Product Type	Measurement Mode	Applications, Features, and Benefits
Bossart Analytics	Calibration-Model.com	Development of NIR chemometric calibration models as a service	N/A	With this service, NIR-models can be developed without chemometric software on nearly all desktop and mobile NIR spectrometers. Free NIR-Predictor software is included. The user can create analysis result reports with multiple NIR-calibrations at once The complete calibration settings that includes the intellectual property are also available. The developed calibrations are available as perpetual licenses. Applications: Any type of NIR, vis-NIR, or Raman application.
Eigenvector Research, Inc.	Model Exporter 3.5	N/A	N/A	Model Exporter is an add-on tool for PLS Toolbox and Solo that exports models to a stand-alone "predictor" script. Model Exporter includes a simple-to-implement formula to perform model predictions. Add the power of multivariate modeling to a proprietary application or simply apply models in Matlab, Octave, Tcl, or Symbion.
	Solo Predictor 4.0.3	N/A	N/A	A flexible way to use Solo and PLS Toolbox models in an on- or at-line environment. Interfaces options to connect to existing clients and data management systems. Supports Solo and PLS Toolbox standard model types, and instrument standardization developed in the CalTransfer graphical user interface.
	MIA Toolbox 3.0.8	N/A	N/A	This is an add-on for PLS Toolbox and Solo that brings chemometrics to hyperspectral image analysis. Allows users to load, manipulate, and analyze multivariate images in the analysis graphical interface.
	PLS Toolbox 8.8.1	N/A	N/A	A collection of essential and advanced Matlab routines that contain the tools required to explore their data and build predictive models.
	Solo 8.8.1	N/A	N/A	A standalone data science and chemometrics package that employs PLS Toolbox graphical user interfaces for quickly managing and analyzing data.
Ocean Insight	OceanView 2.0 Software	Operational and computational software package	N/A	A powerful new version of the OceanView spectroscopy software, with a smooth, intuitive graphical user interface (GUI) and faster, more stable data acquisition and processing. The enhanced GUI has visual contrast to reduce eyestrain and provides a friendlier experience. It is compatible with 32-/64-bit operating systems running Windows, MacOS or Linux.
S.T.Japan-Europe GmbH	Databases of Designer Drugs, New Psychoactive Substances, Legal Highs, Research Chemicals, Doping and other Illicit Substances	Spectral database	NA	The databases are compatible with the software of all major instrument manufacturers. These new spectra libraries of new psychoactive substances were issued in cooperation with the German customs laboratory. The substances are among the most recent psychoactive substances in the market seized by German customs authorities.
Thermo Fisher Scientific	NanoDrop	QC software for the NanoDrop OneC spectrophotometer	N/A	This product enables measurement of highly concentrated solutions without dilution. Analyze 0.5–2.0 µL samples without the need for cuvettes or capillaries. Measure samples without needing to know the sample concentration, Quantify up to 550 AU with automated short-path-length adjustments. Run on-board chemometric methods. Simplify chemometric method development with Thermo Scientific TQ Analyst Software. Deploy methods directly to Thermo Scientific NanoDrop OneC UV-vis spectrophotometers around the world, Achieve pass/fail, and other quantitative results on the factory floor.

Continued on Page 44

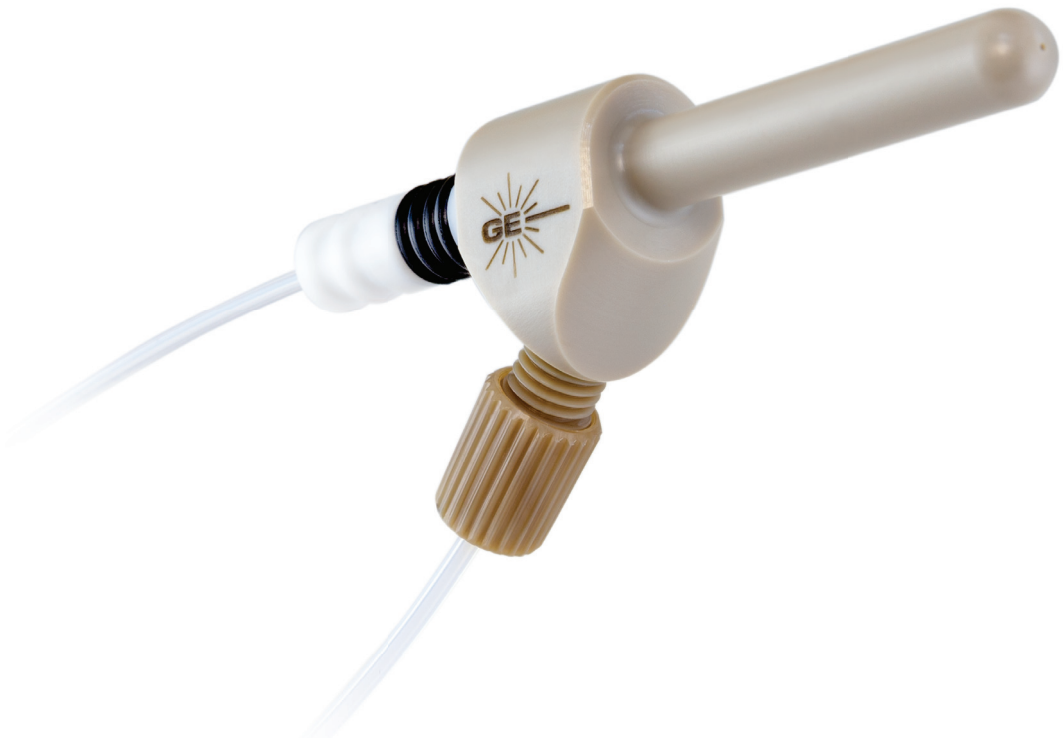
(including lubrication, pharmaceuticals, and environmental markets). In contrast, PS Analytical focuses on mercury monitoring, with a continuous operations profile.

PS Analytical manufactures mercury monitors for water and air monitoring. Features include automatic self-calibration, ultralow limits of detection (LOD), and low reagent usage.

Thermo Fisher displays a new ICP-OES spectrometer with enhanced capabilities over previous models.

See Table II for listings of atomic spectrometers.

High Performance Inert Nebulizers



Samples with residual hydrofluoric acid (HF) require an inert nebulizer made of PEEK, PFA or alumina - glass or quartz nebulizers are not suitable for these sample matrices.

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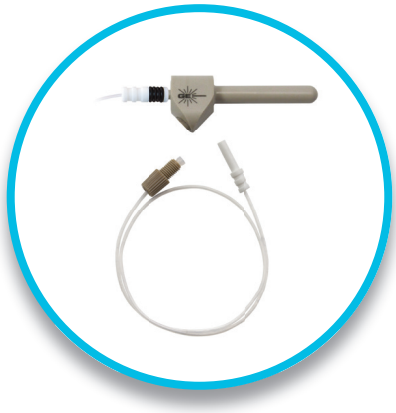
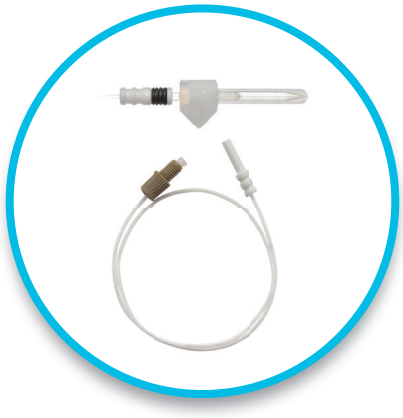
To get the best performance out of your ICP-OES or ICP-MS choose the nebulizer best suited to your instrument and sample needs:



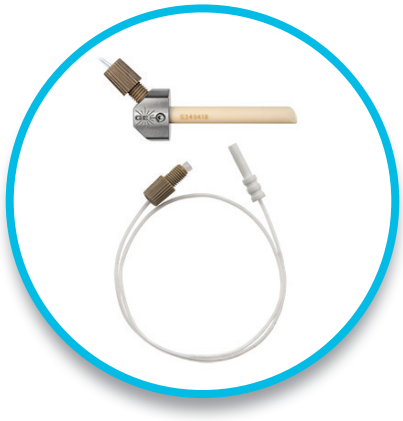
DuraMist Concentric Nebulizer:

Made of PEEK it is an economical inert nebulizer ideally suited to ICP-OES for high sensitivity and excellent short-term precision with the highest tolerance to dissolved salts of any concentric nebulizer.



OpalMist Concentric Nebulizer:

Made of high-purity PFA, perfect for ICP-MS in ultra-trace, high precision analyses of alkalis, organics and samples containing a high concentration of HF. The self-aspiration properties of the nebulizer eliminate the need for peristaltic pump tubing that can be a source of contamination.



VeeSpray Nebulizer:

Made of high purity Alumina grade ceramic, this parallel path nebulizer is virtually unblockable and provides the best tolerance to large particulates and abrasion-resistance.

Learn more at: www.geicp.com/inert-nebulizer

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TABLE IX: Software products (continued)

Company Name	Product Name	Product Type	Measurement Mode	Applications, Features, and Benefits
Tornado Spectral Systems	Spectral-Soft 3.0	Embedded prediction engine	N/A	A key update of the product's instrument control software is an embedded prediction engine supporting the widely used SIMCA. Its *USP* calibration model format offers users stand-alone operation for continuous manufacturing. With software functionality being targeted to Raman analysis, Tornado provides a well-balanced solution that contains great power hidden beneath a simple interface. Many new features and improvements are included.
Unity Scientific	UCal 4	Calibration software	N/A	UCal 4 is a complete chemometric package for the development of high-performance quantitative and qualitative models for Unity NIR instruments. UCal 4 includes advanced algorithms and graphical displays that enable non-chemometricians to create robust and powerful models. UCal 4 also includes population structuring routines, including the patented Condense algorithm to manage large historical datasets, and monitor validation programs to evaluate models. A versatile file conversion utility allows the transfer of calibrations from other manufacturers.

Imaging

The products listed under imaging are all cameras, with and without microscopes. The key improvements are around sensitivity and, more often, speed, which is crucial for these systems, enabling larger areas to be imaged, and a wider range of applications. This is true regardless of spectral range (X-ray to IR).

Andor provides an X-ray camera (Balor-X) that combines a large 16.9 megapixel sensor with the fast readout speed of sCMOS technology, giving 54 FPS at full frame.

Dino-Lite Scopes provide digital imaging microscopes with video interfacing to a PC or Mac.

Edax offers what it is marketing as the fastest EBSD camera on the market, the Velocity Camera Series, offering high-speed EBSD mapping with the best indexing performance on real world materials.

HySpex industrial hyperspectral imagers are fast, flexible, robust, and repeatable, with spectral resolution of two bands, capturing 4X more light.

Nireos provides imaging using a Fourier-transform approach. This approach gives very high sensitivity in a small and light instrument. Spectral resolution is exceptional: <1 nm at 400 nm wavelength. It captures images in a static regime.

Olympus Corporation of the Americas enables measurement and observation of a variety of materials with interactive zoom and guaranteed high- and low-magnification accuracy and precision using a single instrument.

Photonis Scientific provides a single-photon-counting camera with nanosecond time-stamping and <10 µm spatial resolution. Mantis3 consists of a Timepix3-based visible light camera coupled to a Cricket, containing a high-end image intensifier.

Princeton Infrared Technologies offers a compact SWIR–visible camera that supports the 95 FPS frame rate at megapixel resolution with no ITAR restrictions, with high resolution (1280 x 1024 pixels) SWIR imagery.

Sierra-Olympic provides a mid-IR imaging camera with the smallest, lightest, most power-efficient camera in the Ventus product line, offering continuous zoom, one-touch autofocus, advanced image processing, and several other features

See Table III for listings of imaging devices.

TABLE X: UV-vis products

Company Name	Product Name	Product Type	Applications, Features, and Benefits
Edinburgh Instruments	DS5 Dual Beam	Dual-beam UV-vis spectro-photom-eter	A high performance dual-beam instrument suitable for many analytical applications where accuracy and precision measurements are key to results. Utilizing a dual lamp and Czerny-Turner configuration monochromator, it features a compact, high-throughput optical system that ensures impressive spectral performance. Additional benefits include stray light, baseline flatness, wavelength and photometric accuracy, and reproducibility. Applications include nanotechnology, materials research, environmental science, analytical science, quality control, drug discovery, and bioscience.
Essent Optics Ltd	Photon RT spectropho-tometer for coaters	UV, visible, NIR, and mid-IR	Please see the Mid-IR table for the product details.
McPherson	Deep ultraviolet absorbance detector	Deep UV detector	McPherson's deep-UV detectors work from 120 nm in the deep UV up to the visible region. Compatible flow cells are available with three different path lengths and specials can be manufactured to the application. Works with both gas- and liquid phase samples. Deep UV absorbance is enabled by vacuum-compatible flow cell assemblies. These enable researchers to operate with crystalline fluoride windows at very short wavelengths. The spectrometer used to disperse the spectrum and digital camera used to collect signal also exist as standalone products or can be used together with VUVAS material characterization systems.
	Vacuum UltraViolet Analytical Spectro-photometer (VUVAS)	Deep UV and vacuum UV spectro-photometer	Full motorization and computer control of the goniometric sample chamber is the new feature of this system. This allows theta-2-theta measurement of coating, rocking curves, and, with McPherson software, the ability to test the efficiency of diffraction gratings and other dispersive samples very quickly.
Ocean Insight	Ocean HDX-XR	HDX-XR spec-trometer	Ocean Insight has an extended-wavelength range version of its high-definition optics spectrometer. The new Ocean HDX-XR uses optimized optical bench components, specialized materials, and precision engineering to maximize optical resolution, increase throughput, reduce stray light (>3 AU), and maintain thermal stability (±1.0 pixels from 0–40 °C). The Ocean HDX-XR has a 10 µm slit, and dual blazed grating that extends wavelength response from 200 to 1100 nm.
Shimadzu Scientific Instruments	UV-1900i	UV-vis spectro-photom-eter	This spectrophotometer provides high resolution, low stray light, an ultrafast scan function, and an easy-to-use interface. A spectral evaluation function automatically determines whether data satisfy specified criteria, while real-time data transfer simplifies operation. Software includes compliance with electronic records and electronic signature (ER/ES) regulations. Applications include R&D and QC in markets such as foods, pharmaceuticals, life sciences, chemistry, electronics, and academic research and teaching settings.
	UV-2600i/2700	UV-vis spectro-photom-eters	These double-beam spectrophotometers are true research-grade instruments, and have selectable bandwidths to comply with requirements of regulated laboratories and high-end research. They can measure up to 8 abs, and have a wavelength range expandable to the NIR. They provide multiple measurement modes, including photometric, spectrum, quantitation, kinetics, time course, and bio-methods. They include enhanced security functions, and can be equipped with accessories and software programs to address specific applications. Applications include analysis of band gap, optical coatings, thin films, biological samples like DNA and proteins, and routine work associated with UV-vis spectroscopy.
	UV-3600i Plus	UV-vis-NIR spectro-photom-eter	This spectrophotometer is equipped with double grating monochromators, and can achieve ultralow stray light levels, constant optical resolution of 0.1 nm or lower in the U and visible region, and 0.4 nm in the NIR region. The wavelength range is 185–3300 nm, and is suitable for all kinds of samples. It features a large sample compartment, multiple measurement modes, and can be equipped with a variety of accessories, including autosamplers. Applications include haze analysis, band gap analysis, photovoltaics, coatings, and optical component characterization.
	SolidSpec 3700i/3700i DUV UV-vis-NIR	UV-vis-NIR spectro-photom-eters	The SolidSpec-3700i and SolidSpec-3700i DUV (Deep-UV) spectrophotometers can measure from deep-UV to visible and up to 3300 nm in the near-IR. A large sample compartment allows analysis of large solidS without cutting them. They come outfitted with integrating spheres or a direct detection unit (DDU) can be installed for direct transmittance measurements. With the available automatic X-Y stage, a large sample can be measured and users can assign sampling points in the software.

TABLE XI: X-ray products

Company Name	Product Name	Product Type	Applications, Features, and Benefits
Elvatech Ltd.	ElvaX RoHS	XRF instrument	Special features of this product include compact size (280 x 385 x 200 mm), high speed, accuracy, 5 in touch-screen display, 5 position collimator from 1 to 10 mm, 6 h continuous operation battery, automatic Cl correction, correction for thickness of plastics, the ability to work under the control of an external PC, and an integrated printer. Applications include the analysis RoHS directive for Pb, Hg, Cd, Cr, Br.
IXRF Systems	Atlas	Micro-XRF spec-trometer (μXRF)	The Atlas Micro-XRF spectrometer (μXRF) creates a new world of X-ray mapping and automation. The Atlas boasts the largest chamber volume and detection area (150 mm^2), as well as the smallest spot size (5 μm) available on the market. Additionally, the Atlas is complemented by the most comprehensive software suite, including multi-point analysis, unattended automation, in-depth feature and image analysis, and unprecedented mapping and reporting features.

Mass Spectrometry

Size and sensitivity were major themes for the mass spectrometry (MS) offerings. There is also a unique analyzer specific for honey (Elementar). This category has responded to the general instrumental trend toward smaller laboratory settings with the same or higher sample loads, demanding space-saving solutions. A major advantage of MS over other techniques is extreme sensitivity. Downsizing the system allows for smaller vacuum systems (pumps), due to decreased volume. This trend will continue as the importance of MS in many fields continues to grow.

Elementar Analysensysteme GmbH uses high temperature to generate ions, whose isotope ratios are subsequently detected by MS, to determine adulteration of honey.

Excellims combines its mobility technology with a miniaturized ion-trap mass spectrometer to create a small-footprint, miniaturized instrument. They also offer an autosampler accessory.

Hiden provides a variety of configurations of their mass spectrometers, each promoted and optimized for a different application.

Ionicon offers two new time-of-flight (TOF) mass spectrometers with extremely high sensitivities and correspondingly low limits of detection.

JEOL provides an imaging matrix-assisted laser desorption ionization (MALDI)-TOF/TOF mass spectrometer with ultrahigh mass-resolving power and an optional MS/MS with unit-mass precursor selection for imaging samples that are not perfectly flat.

See Table IV for listings of mass spectrometers.

Mid-IR

Mid-IR spectroscopy itself is relatively mature, with sensitivity and signal-to-noise well within the needs of most laboratories. Expansion of mid-IR tools is being explored through multirange capabilities (long possible, but being simplified) and software tools (such as remote operation and cloud processing). There is still a need for inexpensive, task-specific analysis, as the speed, cost, and selectivity of mid-IR spectroscopy remain its strongest assets.

Brightspec brings a new type of spectroscopy to the analytical world. The isoMRR spectrometer measures rotational spectra to identify species based on differences in their three-dimensional mass distributions, and brings a much higher level of selectivity to isomer and isotope analysis than MS.

EssentOptics has the widest wavelength range (185–5200 nm) in a single instrument. Transmission and absolute reflection measurements at variable AOI's and polarizations are built-in capabilities.

Reflex Analytical provides capability to sample, and measure up to 24 samples of biodiesel fuel in one run.

See Table V for listings of mid-IR spectrometers.

NIR

The NIR category shows some strong trends from multiple vendors. First, smaller, portable instruments are now the mainstay (Avantes, Galaxy, Ocean Insight, and Spectral Evolution, for example). Second, micro electro mechanical systems (MEMS) continue to appear as a key solution, due to lower cost and simple construction (such as in instruments from SouthNest and Ocean Insight). Third, as noted in the mid-IR section, multirange capability is extending the applications space (see Wasatch and Spectral Evolution). All three of these trends have been identified in previous years, as this field appears to be converging on a small number of attributes essential to the task-oriented tools being launched.

Avantes provides a small form factor, high resolution, high sensitivity uncooled InGaAs spectrometer. USB connection makes it easy to integrate into other devices, including original equipment manufacturer (OEM) and handheld applications. This product is well suited for various applications, including food analysis, security monitoring, and the recycling industry.

Galaxy Scientific provides a compact, portable, and high-performance FT-NIR spectrometer with a triggered fiber optic probe for laboratory and field, and a built-in probe holder. This spectrometer is designed from the ground up to offer the industry a new kind of NIR analysis solution.

EssentOptics provides coverage of NIR, UV, visible, and mid-IR (185–

TABLE XII: Accessories

Company Name	Product Name	Product Type	Measurement Mode	Applications, Features, and Benefits
Alliance Corp	KeepSafe Pouch	Protective pouches	N/A	Non-abrasive pouches that are perfect for the safe transit of items with delicate surfaces. Made from ultrasoft spun-laced polyester. The openings are available with an offset, fold-down flap, and reclosable flap. There are no glue or other chemicals used in the manufacturing process. Available from 1 in x 1 in to 8 in x 8 in. Made in the United States.
Art Photonics	Transflexion (Dual Pass) Fiber Probe	Transflection fiber probe	Transflection	The Transflexion fiber probes have a rugged industrial design. All optical parts are made from sapphire with AR coating. Can be used with any spectrometer or photometer, and are compatible with process interfaces to be cleanable, and to enable reaction monitoring in laboratory, pilot plant, and run full automated process control.
	Raman Fiber Probe	Raman fiber probe	Raman scattering	The Raman fiber probe can be used with any Raman spectrometer. Featuring multi-wavelength excitation (630–785 nm) and single-wavelength excitation (532 and 785 nm), the Raman probe allows a user to analyze spectra in fingerprint (800–1800 cm^{-1}) and high wavenumber (2800–3800 cm^{-1}) spectral ranges using different lasers. They are cleanable and enable reaction monitoring in laboratory, pilot plant, and running full automated process control.
	NIR-Raman Combi Fiber Probe	Combined NIR and Raman fiber probe	Transmission and Raman scattering	This unique combined fiber optic probe (NIR + Raman) provides simultaneous measurements for both methods at the same point, to measure process and product characteristics in real time. The unique feature of the probe is that NIR and Raman channels can work simultaneously, providing hybrid modeling opportunities that were impossible in the past.
Coherent, Inc	Dual Polarization THz–Raman Probe	THz-Raman probe	Raman scattering	This product simultaneously collects both parallel and cross-polarized Raman signals, giving insight into both chemical and structural properties of the sample, while taking advantage of the wide variety of sample interface accessories (probe, vials, microscope, transmission). The dual polarization design splits the collected signals into two orthogonal polarization states that are coupled into two separate fibers, or a single bifurcated fiber for simultaneous collection.
Galaxy Scientific Inc.	Compact Heated Liquid Sampler	Liquid sampler	Transmission	This compact heated liquid sampler is used with Galaxy Scientific's fiber-based FT-NIR spectrometer to analyze liquid based products' samples. The product features a temperature-controlled fiber coupled main sample chamber, along with a preheating chamber that is designed to hold multiple samples at a time. The compact heated liquid sampler has an easy-to-read 3.2" touch screen interface where the temperature values are displayed and set.
Reflex Analytical Corporation	Four in One XRF Evacuable Pellet Die	Evacuable pellet die	N/A	This product converts a 40 mm die into a 32 mm, 25 mm, or 20 mm die, eliminating the need to purchase four different dies. Using the 40 mm chamber, you can use the appropriate die conversion insert to produce 32 mm, 25 mm, or 20 mm pellets. The 40 mm die is available with or without inserts.
	Ultra-High vacuum flanges and viewports	Ultra-High vacuum flanges and viewports	N/A	This product achieves UHV performance at 10–12 cm^3/s established with fluorocarbon O-ring seals and a differentially pumped vacuum system, by pumping on the differential section with only a mechanical pump, offering a reliable solution to replace and eliminate vacuum seal failures. Several diameters are available.
	Custom UV-vis-NIR cuvettes and cells	Custom cuvettes and cells	N/A	UV-vis-NIR cuvettes and cells are assembled by direct fusion, ensuring resistance to chemical attack and temperature extremes. The selection presents over 150 cuvette and cell types for use in spectroscopy, fluorimetry, calorimetry, polarimetry, cytometry, DNA and protein analysis, blood analysis, dynamic light scattering, and many more applications. Available with fitted covers, plugs, screw caps, anaerobic screw caps, graded seals, and flow through ports. Custom cuvettes and cells are encouraged and available upon request.

TABLE XII: Accessories (continued)

Company Name	Product Name	Product Type	Measurement Mode	Applications, Features, and Benefits
Reflex Analytical Corporation	500 °C Stainless Steel Gas Cell	10 cm High-temperature gas cell	N/A	This 10 cm fixed pathlength stainless steel gas cell can operate at temperatures up to 500 °C . The body is isolated from the mounting plate by a thermal insulator and metal protective enclosure, which prevents heat transfer within an instrument's sample compartment. The cell incorporates a dual-band heater, type K thermocouple, stainless steel ports with 1/4 in Swagelok fittings, and programmable temperature controller. The cell can be configured for breadboard and FT-IR instrumentation.
Savillex	VC Ultra	Acid vapor cleaning system	N/A	Savillex's VC Ultra Acid Vapor Cleaning System uses high purity acid vapors to effectively acid clean-up to 40 microwave digestion vessels and covers in a single run. Customized microwave vessel cleaning racks minimize handling and acid exposure, while preloaded cleaning profiles eliminate the need for method development. The Universal Cleaning Kit enhances the versatility of the VC Ultra, and can be used to clean a variety of other labware used for trace metals analysis.
Spetec GmbH	Precision SY	Syringe pump	N/A	The pump was specially developed for use in equipment where high precision in the microliter and nanoliter range is required when introducing samples or reagents. The mounting plate is tailored to customer needs. No gear box creates much less vibration.
	EasyClick	Compact peristaltic pump	N/A	This new version pump is equipped with a pressure cartridge in which the user simply places the tubing. The cartridge can then be fixed in position by means of a special click-in spring mechanism that also ensures that the tubing is automatically adjusted during pump operation, so there is no longer any need for manual readjustment by the user. The tubing is automatically adjusted during pump operation, with the result being that there is no longer any need for manual readjustment during operation.
Spectral Evolution	Sensaprobe	Hand-held probe	Transmission, reflectance, absorbance, direct energy measurement	The Sensaprobe grip has active feedback, showing the user a picture of the area targeted, indicating when the probe angle is at nadir, noting the angle of the sun, and providing the GPS location The Sensaprobe grip features a tilt-angle sensor, autorangefinder, and camera, to automatically photograph and record field of view of the scanned image.
Tornado Spectral Systems	Opis 35	ATEX Certified class 3B safe laser accessory	N/A	The ATEX-certified class 3B laser safety accessory makes Tornado's HyperFlux PRO Plus Raman analyzer compliant for ATEX Zone 0, providing a solution that alleviates complex and expensive system-level safety protocols. The accessory regulates the HyperFlux Pro Plus laser output to guarantee that no greater than 35 mW of laser power can enter the hazardous location. The accessory is ideal for any ATEX zone application, and extends into many industries, such as fine chemicals, petrochemicals, pharmaceuticals, and liquefied natural gas (LNG).
Wasatch Photonics	RP Var	Raman probes	Raman scattering	These fiber optic Raman probes offer an interchangeable tip for flexible sample interfacing. The standard probe tip can be exchanged for a longer probe barrel, an immersion probe tip, a barrel that accommodates standard ½" lenses, adaptors for coupling to a microscope or scanning stage, or other unique designs. These high NA Raman fiber optic probes are available to be compatible with 405, 532, 633, 785, 830, and 1064 nm excitation, and are matched to f/1.3 Raman spectrometers. The new flexible barrel design accommodates multiple probe tip options, and configurable working distances. This allows the probe to be configured for the application, from immersion use in process, to microscopy or mapping, with focal lengths ranging from 2 to 25 mm.

5200 nm) in a single instrument. NIR is a subsidiary listing for this product; please see the main listing in mid-IR for more information.

Ocean Insight has launched a compact FT-NIR spectral sensor for qualification and quantification of materials from 1350–2500 nm (7400–4000 cm^{-1})

The Si-Ware Neospectra scanner is a hardware- and software-ready device that enables field material analysis applications.

SouthNest Technology Ltd provides an FT-IR and NIR system based on MEMS technology. The larger FT-IR mirror size (mm range) allows more light to enter the system to improve signal quality.

Spectral Evolution has made available two field-capable NIR spectrometers. One has high-resolution, for measuring fine distinctions between similar materials. The other is a heavy-duty field-trans-

TABLE XIII: Components

Company Name	Product Name	Product Type	Applications, Features, and Benefits
Armadillo Sia	Silica/Silica Non Circular Core Fiber	Fiber optics	These optical fibers show the same properties as Optran UV/WF fibers. With good image scrambling and low degradation, the fibers are ideal for astronomy applications. Greater coupling efficiencies are provided when used with diode lasers than circular fibers. NCF fibers have square or rectangular shape, offering advantages due to providing maximum packing density for input and output.
Cobolt, a part of Hübner Photonics	08-NLD 785nm ESP	Laser	The spectral purity of the 08-NLDM 785 nm ESP laser is >60 dB as close as 0.3 nm away from the main laser peak. Enhanced spectral purity (ESP) is a desired performance specification for low frequency Raman applications, and defines how well the side modes are suppressed relative to the main laser peak.
Eblana Photonics Ltd.	EP-DM series	Lasers	Eblana's Discrete Mode (DM), DFB-like diode lasers are designed to deliver stable and precise lasing performance in the NIR–MIR range, for a wide range of applications. The proprietary discrete mode (DM) laser platform allows production of custom laser designs at any wavelength in the NIR and MIR. Eblana's lasers comprise of narrow line-width (2 MHz, down to 100 kHz), high SMSR (>40 dB) and tunability (2 nm). With an available wavelength range: 657–2350 nm, applications include gas sensing, biosensing, and LIDAR.
Electro-Optics Technology	Tornos	Compact isolator	The Tornos compact isolator offers compact design in a wide range of models, ≥95% transmission, and ≥33 dB isolation. Applications include Raman spectroscopy, DNA sequencing, imaging, environmental sensing, mapping, microscopy, 3D metrology, and protecting pump lasers in amplified systems.
MKS Spectra-Physics	InSight X3+	Tunable laser	The InSight X3+ is built on Spectra-Physics' platform for maximum performance and reliability. With a repetition rate of 80 MHz, this laser provides broadband tuning from 680–1300 nm, with >3 W of output power at 900 nm (a 50% increase in power over the previous generation), >2.7 W at 1000 nm, >2.4 W at 1100 nm, and high average power across the entire tuning range, with ultrashort pulses and integrated dispersion pre-compensation. It is a hands-free design, and includes a synchronized 1045 nm output that can be used in combination for CARS and SRS.
OPCO Laboratory, Inc.	Echelle Grating, High Resolution	Echelle grating	These high-resolution echelle gratings are differentiated by their high efficiency and low scatter. New features (improved efficiency and low scatter) originate in their state-of-the art ruling engine for creating the master ruling. The elimination of mechanical errors and incorporation of the latest vibration, thermal, and motion control technology into the engine design enable very repeatable groove structures, resulting in the benefits mentioned above. Applications include laser induced breakdown spectroscopy (LIBS), Raman spectroscopy, and fluorescence spectroscopy.
Spectrolight Inc.	FWS Poly Laser Version	Flexible wavelength selector (adjustable optical filter)	This is a compact fully automated flexible wavelength selector—an opto-mechanical device that allows simultaneous center wavelength and bandwidth adjustment, spanning the entire visible spectrum with a circular uniform aperture. The FWS Poly-LV provides advantages over existing filter and filter wheel technologies (such as AOTF and liquid crystal filters), with performance and cost advantages, including high transmission, steep spectral edge, and high out of band blocking. This is a new version of the existing FWS Poly device. The previous model is compatible with various light sources (including lasers), while the new models are compatible with lasers only. The maximum beam size for the laser version is 3 mm while the standard version is 10 mm. The laser version is also the cost-effective option.
UniKLasers Ltd.	Solo640 series	Solid-state diode lasers	These lasers include have extended power and wavelength stability, delivering more than 8 h of non-stop operation along with impressive output powers of up to 1000 mW. These have a remote-control function that allows users to switch a laser on/off and adjust output power through a PC, as well as conduct remote diagnostics for service, maintenance and training.

portable spectrometer, for use in rugged environments.

Wasatch Photonics has two new, but similar, spectrometers intended for OEM use. They differ in the wavelength range covered; the NIR-only instrument covers 900–1700 nm, while the vis-NIR spectrometer covers the range 350–1000 nm.

See Table VI for listings of NIR spectrometers.

NMR

It was only a few years ago that a nuclear magnetic resonance (NMR) spectrometer required a huge, multi-ton superconducting electromagnet to provide a magnetic field that was sufficiently strong and uniform to allow measurement of NMR signals. Then, a few years ago (first showing up in our 2014 annual review), a breakthrough occurred: Tabletop NMR instruments were demonstrated at Pittcon, in the form of the PicoSpin series from Thermo Fisher Scientific. These instruments

were based on the development of very high-flux permanent magnets that required no power or cooling water to generate a magnetic field usable for the NMR measurement.

Fast forward another few years, and another breakthrough in NMR measurement technology was presented at this year's Pittcon. Waveguide Corporation showed the world's first handheld, battery-operated NMR analytical instrument, optimized for nonexperts to make decisions in the field at the point-of-use (or point-of-care in medical applications). Applications include authentication of vaccines and biologics, anti-counterfeit, expired or substandard medicine, foods, the petrochemical industry, and medical diagnostics (such as tuberculosis screening and a fast, low-cost, accurate method for the earlier detection of ovarian and other cancers due to the miniaturization of NMR) by a factor of more than 100x. WaveGuide's NMR operates within minutes between wide ambient and sample temperatures, and only requires ~30 µL of sample.

See Table VII for listings of NMR spectrometers.

Raman Spectroscopy

As we examined the current crop of new instrument submissions, we find a strong emphasis on Raman spectroscopy. This was also true some years ago, when handheld Raman instruments were prevalent. This year, we find multiple new or redesigned benchtop instruments (produced by manufacturers such as Horiba, Renishaw, Kaiser, and Thermo Fisher) as well as an array of accessories (see the Accessories section). The growth in Raman spectroscopy is driven by the continued evolution, in both capability and price, of the components (lasers, detectors, spectrographs, and, critically, software), and a response to penetration of this technique into laboratory space traditionally held by Fourier transform infrared (FT-IR) spectroscopy. The advantages of FT-IR (cost, size, and familiarity with and acceptance by laboratory personnel and regulatory agencies) are being eroded, as simpler and more effective Raman spectroscopy devices are released. Solutions to the need to avoid fluorescence or sample surface irregularities are making the tools more useful in a wider range of laboratories. It is also telling that almost all of the major Raman instrument vendors provide on-line training; this has the impact of creating an informed user base, and also evoking confidence that the vendor has subject matter expertise. This is not orthogonal to product development; it is critical to the companies' messaging.

We expect Raman systems will continue to evolve in two main directions. Handhelds have already penetrated the security market and law enforcement, as well as loading dock quality control (QC). Tabletop units are evolving new imaging tools, better, smarter software, and automation. The new components point the way to new spectrometers, as each vendor seeks an advantage in performance or the elusive "ease of use."

AcuTech Scientific Inc. provides lightweight, small, handheld Raman spectrometers, with validated libraries available. The Acuscan1350 Gemstone Identifier is specialized in accurate and easy gemstone and mineral identification, and includes a turntable for a 360° scan of a large size gemstone.

Agilent provides a handheld, spatially-offset Raman spectroscopy (SORS) system for QC testing of pharmaceutical, biopharmaceutical, and nutraceutical raw materials through transparent and non-transparent containers.

B&WTek recently presented Raman spectrometers for the identification of controlled substances, and also for identification of analytes contained in visually opaque containers. They also launched the STRam-1064, which can identify material inside visually opaque barriers such as plastic bottles and paper bags.

Edinburgh Instruments provides a truly confocal design unique to the market, and offers uncompromised spectral resolution, spatial resolution, and sensitivity. The Ramacle RM5 Raman Microscope offers a variable slit and multiple position adjustable pinhole for higher image definition, better fluorescence rejection, and application optimization. The RM5 builds on the expertise of robust and proven building blocks, combined with modern optical design considerations. It has a focus on function, precision and speed.

Horiba presents the LabRam Soleil, which boasts ultrafast Raman imaging (100 times faster imaging). This is the first multi-modal Raman microscope designed to include UV-vis and NIR imaging.

Kaiser Optical Systems supplies a high-resolution, research-grade Raman spectrometer on a portable platform for process development monitoring and control. A single analyzer can collect Raman data from four channels, addressable by fiber-optic probes, and is capable of direct in situ measurements, without needing custom sampling devices.

Metrohm showed the Mira handheld Raman spectrometer, which can identify material in a container with opaque walls.

Ocean Insight (previously Ocean Optics) has a high-sensitivity, 785 nm Raman spectrometer, providing low limits of detection for trace-level materials identification.

Thermo Fisher is showing three models of Raman microscopes: a basic unit, and two intended for special applications, one for real-time analysis and one with automated setup and control features.

Wasatch Photonics presents two Raman spectrometers, one an extended-range Raman spectrometer designed to measure out to 3500 cm^{-1}. The other is similar, but features

a fully integrated 350 mW multimode laser that is both powered and controlled through the spectrometer.

WITec's Truly Confocal Raman microscope offers excellent spectral resolution, spatial resolution and sensitivity.

See Table VIII for listings of Raman spectrometers.

Software

As described in the introduction, software appears to be on the cusp of a major evolution. Vendors have all identified the trend in many laboratories of downsizing staffing, against a continued increase in sample loads. This means a single worker must be able to move between multiple instruments without major barriers. Easy sample transfer and shallow learning curves via workflow software are becoming common needs. As we said earlier in this review, vendor announcements often bury the these features under hardware developments. It becomes immediately apparent, however, when you watch instrument demonstrations that the demonstration is driven by software ("See how easy this is?"). This trend is leading to many changes in the user interface and user experience (UI and UX), as we pointed out in last year's analysis of trends we were beginning to see: cloud storage, multi-instrument data integration and, slowly, but inevitably, machine learning, where a computer becomes a true laboratory partner. It is an exciting time for both users and vendors.

Software, in the context of this review, consists of several different, albeit related, types of products, including actual computer programs, compilations of spectra, databases, and collections of chemometric calibration models.

Bossart offers NIR calibration development as a service.

Eigenvector has enhanced and upgraded the routines in most of their core products, including PLS Toolbox, Solo, Solo Predictor, MIA Toolbox, and Model Exporter.

Ocean Insight provides a powerful new version of its OceanView spectroscopy software, with a smooth, intuitive graphical user interface (GUI), and provides faster, more stable data acquisition and processing.

S.T. Japan-Europe GmbH provides spectral databases of illicit drugs, including phenethylamine, synthetic cannabinoids, cathinones, piperazine, tryptamines, mephedrone, steroids, and others.

Thermo Fisher Scientific provides software for its NanoDrop Instrument that simplifies the operation, and extends the capabilities of the instrument.

Tornado Spectral Systems presents a key update of its instrument control software features that offer users standalone operation for continuous manufacturing.

See Table IX for listings of spectroscopy software.

UV-vis

Some entrants in the UV-vis category could have been included under software (Thermo Fisher Scientific) or NIR (see that section for the multirange capabilities). While most emphasize small size and moderate performance, Edinburgh is showing a high-performance unit.

Edinburgh Instruments provides a high-performance dual beam instrument suitable for many analytical applications where accuracy and precision measurements are key to results. Utilizing a dual lamp and Czerny-Turner configuration monochromator, the instrument features a compact, high throughput optical system, which ensures impressive spectral performance.

EssentOptics provides coverage of UV, visible, and NIR and mid-IR (185–5200 nm) in a single instrument. Please see the main listing in mid-IR for more information.

McPherson provides deep ultraviolet and vacuum ultraviolet spectrometers with capabilities of vacuum-compatible flow cells, and a motorized and computer-controlled sample chamber.

Ocean Insight announces an extended-wavelength-range version of its high-definition optics spectrometer. The new Ocean HDX-XR uses optimized optical bench components, specialized materials and precision engineering to maximize optical resolution, increased throughput and reduced stray light (>3 AU).

Shimadzu launched four UV-vis spectrometers. The UV-19001 provides high resolution, low stray light, an ultrafast scan function, and an easy-to-use interface. The UV-26000i/2700i double-beam spectrophotometers are true research-grade instruments, and have selectable bandwidths to comply with requirements of regulated laboratories and high-end research. The UV-3600i Plus is equipped with double grating monochromators, and can achieve ultralow stray light levels, constant optical resolution of 0.1 nm or lower in the UV and visible region, and 0.4 nm in the NIR region. The SolidSpec-3700i and SolidSpec-3700i DUV (deep-UV) can measure from deep-UV to visible and up to 3300 nm in the near-IR.

Thermo Fisher Scientific provides software for their NanoDrop Instrument; see the Software section for details.

See Table X for listings of UV-vis spectrometers.

X-ray

The X-ray category is small this year, preventing a general statement.

Elvatech Ltd. provides an instrument to check for compliance to restriction of hazardous substances (RoHS) specifications.

IXRF Systems provides the Atlas Micro-XRF spectrometer (μXRF) that is used for X-ray mapping and automation.

See Table XI for the listing of X-ray spectrometers.

Accessories

This is our largest pool of submissions. Accessories are developed

around specific needs or shortcomings in existing tools. Fiber optics (such as those manufactured by Art Photonics and Wasatch) provide simplicity in sampling. Cuvettes hold samples (Reflex) and hand tools are common (Reflex). Other tools address gas handling (Spetec, Reflex). An interesting item here is a form of packaging: pouches for transport of delicate items (Alliance).

Alliance Corp provides protective pouches for optics (lenses, mirrors, filters) to keep their surfaces pristine and free from scratches.

Art Photonics offers three different fiber probes: a transflection probe for visible and NIR applications, a Raman fiber probe, and a combined (transflection and Raman) capability.

Coherent provides a Raman probe that can simultaneously collects parallel and cross-polarized signals for both Raman and terahertz probes.

Galaxy Scientific has a new liquid sampler that is used with fiber based FT-NIR spectrometers to analyze samples of liquid-based products. The sampler features a temperature-controlled fiber (coupled main sample chamber), a preheating chamber, and an easy to read 3.2-in touch screen interface where the temperature values are displayed and set.

Reflex Analytical offers several different spectroscopic accessories:

- a four-in-one XRF pellet dies for various pellet sizes
- fluorocarbon O-ring seals and differentially pumped vacuum system that achieve UHV performance at 10–12 cm^3/s
- UV-vis/NIR cuvettes and cells, assembled by direct fusion, ensuring resistance to chemical attack
- high-temperature gas cells with 10 cm pathlength.

Savillex provides an acid-vapor cleaning environment, capable of cleaning multiple devices simultaneously.

Spetec now provides new syringe pumps (for precision cell filling) and peristaltic pumps (for injecting samples into flow-through cells).

The Spectral Evolution Sensaprobe is not just a holder for the probe; it also provides active feedback, so you know exactly where on the sample your spectrum is coming from.

Tornado Spectral Systems has an ATEX certified laser safety accessory that provides a safe environment around Class 3B lasers.

Wasatch Photonics offers Raman probes that are highly configurable. These probes offer interchangeable tips and adapters for coupling to a microscope or stage, are available for 405, 532, 633, 785, 830, and 1064 nm excitation, and are matched to f/1.3 Raman spectrometers. Tip options have configurable working distances. Thus, the probe can be configured for the application, from immersion use to microscopy or mapping, with focal lengths ranging from 2–25 mm.

See Table XII for listings of accessories.

Components

Component manufacturers both lead and follow instrument vendors. New lasers (such as those produced by Eblana, MKS Spectra-Physics, Cobolt, and UniKLasers), new gratings, and optics (produced by Electro-Optics, OPCO, and Spectrolight) often relate to the larger world of Raman spectroscopy and related fields, responding to specific needs, and driving future product developments.

Armadillo Sia offers optical fibers with noncircular cross sections.

Cobolt provides lasers with exceptionally high spectral purity. Purity of this laser is >60 dB as close as 0.3 nm away from the main laser peak. Enhanced spectral purity (ESP) is a critical specification for low frequency Raman applications.

Eblana Photonics provides custom discrete-mode diode lasers with stable and precise lasing performance over the whole the mid-IR and ZAZ wavelength ranges.

Electro-Optics Technology provides wide range of electro-optic isolators to cover many different wavelength ranges, featuring ≥95 % transmission and ≥33 dB isolation.

MKS Spectra-Physics presented a new tunable laser, with a repetition rate of 80 MHz, and broadband tuning from 680–1300 nm, with >3 W of output power at 900 nm (a 50% increase in power over the previous generation).

OPCO Laboratory's echelle gratings are differentiated in the marketplace by their high efficiency and low scatter.

Spectrolight has a variable filter that allows center wavelength and bandwidth adjustment, spanning the entire visible spectrum. The previous model is compatible with various light sources, while the new models are compatible with lasers only. The maximum beam size for the Laser Version is 3 mm.

UniKLasers Ltd. provides solid-state diode lasers (SSDL); their specifications include advanced remote control operation (GUI),and they deliver more than 8 h of non-stop operation, along with output powers of up to 1000 mW.

See Table XIII for listings of components.

Howard Mark serves on the Editorial Advisory Board of *Spectroscopy* and is a coauthor of the "Chemometrics in Spectroscopy" column. He also runs a consulting service, Mark Electronics, in Suffern, New York. **Michael S. Bradley** also serves on *Spectroscopy's* Editorial Advisory Board and is a Product Manager at Thermo Fisher Scientific in Madison, Wisconsin. Direct correspondence to SpectroscopyEdit@mmhgroup.com ●

Multi N/C analyzers

Analytik Jena's multi N/C series of analyzers are designed for surface and wastewater investigations in the environmental sector, and high-purity water in the semiconductor or pharmaceutical industry. According to the company, the instrument's corrosion-free Focus-Radiation nondispersive infrared (NDIR) detector has a measuring range from 0 to 30,000 mg/L TOC without sample dilution.

Analytik Jena US, Upland CA.
www.analytik-jena.us/products/sum-parameter-analysis/toctnb-analysis/multi-nc/

Inert nebulizer guide

Glass Expansion's *High Performance Inert Nebulizers Guide* reportedly details the company's high-performance inert nebulizer designs. According to the company, the guide provides help in selecting a nebulizer that is best suited to a laboratory's requirements.

Glass Expansion, Inc., Pocasset, MA.
www.geicp.com/inert-nebulizer

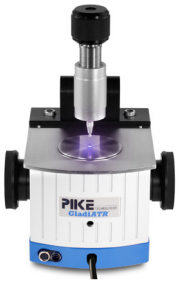
Raman spectrometer

The QE *Pro*-Raman+ high-sensitivity 785 nm Raman spectrometer is designed to provide low limits of detection for trace-level materials identification. According to the company, the spectrometer provides clean, sharp, and stable Raman signatures from 105 cm^{-1} to 3000 cm^{-1}.

Ocean Insight,
Largo, FL.
www.OceanInsight.com

ATR accessory

The GladiATR Illuminate diamond ATR accessory from PIKE is designed for the analysis of photocuring or the solidification of liquid resins upon exposure to light. According to the company, the accessory irradiates the sample from underneath through the diamond ATR element, overcoming issues with nonuniform sample thickness, and influences of sample absorption.



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

Benchtop pellet press

REFLEX Analytical's benchtop pellet press is designed for the compression of powdered materials using standard or custom die sizes. According to the company, the compact, hand-operated press can be used anywhere in the laboratory, and requires very little bench space and no fixed mounting.

REFLEX Analytical Corporation,
Ridgewood, NJ.
www.reflexusa.com/pelletpress.html

Scanning multi-element process coatings analyzer

Rigaku's NEX LS energy dispersive X-ray fluorescence (EDXRF) scanner is designed to perform multi-element composition, coat weight, and coating thickness analyses for web and coil applications. According to the company, the analyzer enables real-time coating analysis (for example, Cr, Ti, V, Mn, Ni, and Zr) on metal substrates.

Rigaku Corporation, Tokyo, Japan.
www.rigakuedxrf.com/xrf.php

Microwave digestion system

The CEM MARS 6 microwave digestion system is designed to digest challenging samples for trace metals analysis. According to the company, the system has hundreds of preprogrammed methods and vessel options for high throughput and difficult samples.

CEM Corporation,
Matthews, NC.
www.cem.com/mars6

Raman spectrometer

Raman spectrometer
The Mira P Raman spectrometer from Metrohm is designed for material varication in regulated industries. According to the company, the spectrometer is barely larger than a smartphone, and provides results in seconds.

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

Photo Credit: adobestock.com/selensergen

PRODUCTS & RESOURCES

Microwave digestion

Milestone's UltraWAVE microwave digestion system uses the company's single reaction chamber technology for metals digestions. According to the company, the system uses a single pressurized vessel for all samples, allowing or simultaneous digestion of up to 22 samples. The system reportedly can accommodate a maximum temperature of 300 °C and pressure of 199 bar.
Milestone, Inc., Shelton, CT; www.milestonesci.com/ ultrawave

Acid vapor cleaning system

Savillex's VC Ultra acid vapor cleaning system is designed to acid-clean up to 40 microwave digestion vessels and covers in a single run. According to the company, customized microwave vessel cleaning racks minimize handling and acid exposure, and pre-loaded cleaning profiles eliminate the need for method development.
Savillex, Eden Prairie, MN. www.savillex.com

Spectrophotometer linearity validation

A set of absorbance references for linearity checking is available from Starna. According to the company, these Certified Reference Materials (CRMs) enable users to demonstrate instrument linearity to meet the requirements of major Pharmacopoeia standards, including the latest *European Pharmacopoeia 10.0 Chapter 2.2.25* and *USP Chapter <857>*.
Starna Cells Inc., Atascadero, CA. www.starna.com

Diamond ATR accessory

Harrick's DiaMaxATR is designed to fit most FT-IR spectrometers. According to the company, the accessory can be used with a variety of sample types, including challenging samples such as extremely hard solids, abrasive powders, and highly corrosive liquids. Optional headed and flow cells are available, along with a force sensor with digital read-out.
Harrick Scientific Products, Inc., Pleasantville, NY. www.harricksci.com

AD INDEX

Photo Credit: adobestock.com/selensergen

FACSS PRESENTS

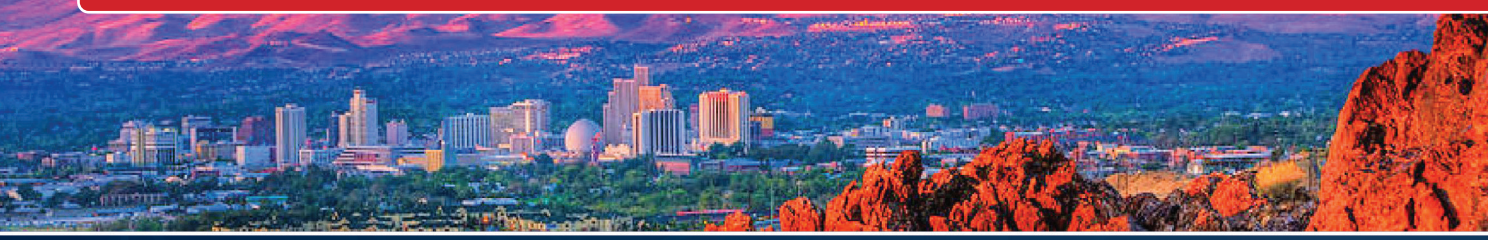
SciX2020

October 11 – 16

Nugget Casino Resort | Sparks, NV

Spark Science at SciX2020

FACSS is continuing to monitor developments related to the COVID-19 pandemic, and planning for SciX in October continues with the well-being of our attendees in mind. We're optimistic that we'll see you in Sparks!



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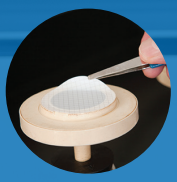
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