Identifying Extractables and Leachables from Polymeric Containers

Corporate Capabilities and Application Notes

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TABLE OF CONTENTS

COLUMNS
8 Molecular Spectroscopy Workbench
Exploration of the Use of Raman Microscopy to the Identification of Extractables and Leachables from Polymeric Containers
Fran Adar
Extractables and leachable are typically studied using chromatographic techniques. This study explores what we can learn by using from using Raman microscopy for such studies.

16 IR Spectral Interpretation Workshop
Infrared Spectroscopy of Polymers, IX: Pendant Ester Polymers and Polycarbonates
Brian C. Smith
We continue our survey of the spectra of carbonyl-containing polymers by looking at cellulose acetate and the economically important polycarbonate Lexan.

SPECIAL FEATURE
Jerome Workman, Jr.
To conclude this four-part series of spectroscopic instrumentation and components, we examine spectroscopy electronics, including printed circuit board (PCB) design and manufacturing, spectroscopy instrument design services, instrument testing services, and the firmware and software aspects of instrumentation.

PEER-REVIEWED RESEARCH
20 Colorimetric Discrimination of Pd^{2+} and Hg^{2+} Ions in Solvent and Solid-Film State Using Organic Acid-Assisted Green Synthesized Silver Nanoparticles
Kaiyu Zhang, Yuxin Sang, Qinxing Sun, and Weina Li
By using green synthesized AgNPs modified by chitosan and organic acid, a simple, cost-effective, and highly selective onsite colorimetric detection method for Pd^{2+} and Hg^{2+} ions was developed.

CORPORATE CAPABILITIES
32 Alluxa 33 LECO 34 GFS Chemicals 36 Harrick Scientific Products, Inc. 38 Jasco 40 Ocean Insight 42 PIKE Technologies, Inc. 44 Moxtek Inc. 45 REFLEX Analytical Corporation 46 Spellman High Voltage Electronics Corporation 47 WITec GmbH

APPLICATION NOTES
48 Analytik Jena 49 Ocean Insight

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The use of Raman microscopy to identify extractables and leachables from polymeric containers is assessed in “Molecular Spectroscopy Workbench,” our cover story in this issue of Spectroscopy. Column editor Fran Adar asks the question, “Does it makes sense to employ this approach, rather than liquid or gas chromatography in conjunction with mass spectrometry, for such identification?” The characteristics considered were ease of sample preparation, the minimum quantity of material amenable to analysis, and the quality of the identification. In the study, three sets of centrifuge vials from three different vendors were exposed to a variety of liquids, and then analyzed. Interestingly, although all of the containers tested were made of polypropylene (PP), the compounds that were extracted were not the same.

This issue also presents peer-reviewed research aimed at developing a fast and convenient method for monitoring palladium and mercury, which is important for waste management, environmental protection, and public health. This study is the first to reveal the effect of organic acid on the synthesis of silver nanoparticles (AgNPs) using ultraviolet (UV)-vis spectroscopy. This process allows for the colorimetric discrimination of palladium and mercury ions simultaneously in the solvent and solid-film state in a sensing system, providing a path for simultaneous on-site detection of these metal ions by the naked eye—and another weapon in the ongoing battle against global environmental pollution.

In addition, we present the final installment of our year-long survey of spectroscopy instrument components, with this segment delving into electronics (including printed circuit board [PCB] design and manufacturing), instrument design services, instrument testing services, instrument software, and services. Previous articles in the series, as well as February’s “The Spectroscopy Instrument Components Terminology Guide” supplement, are available on the Spectroscopy website (spectroscopyonline.com).

In “IR Spectral Interpretation Workshop,” Brian Smith continues his survey of the spectra of carbonyl-containing polymers by looking at cellulose acetate and the economically important polycarbonate Lexan.

This is also our annual issue where we provide corporate profiles, application notes, and product profiles. We encourage you to check out those out.

As we close the year, we thank you for your readership and send our wishes for a happy holiday season and a prosperous 2023.
Exploration of the Use of Raman Microscopy to the Identification of Extractables and Leachables from Polymeric Containers

In a follow-up to my February 2020 column, I started a more systematic study of extractables and leachables. Following a suggestion from Mark Witkowski of the FDA, I looked at three sets of centrifuge vials that were exposed to the following liquids in an effort to evaluate the potential of Raman microscopy to identify compounds exiting in polymers under particular conditions: saline, phosphate buffer, water, saline treatment at 100 °C, phosphate buffer treatment at 100 °C, water treatment at 100 °C, ethanol, chloroform, pH 5, and pH 9. Although all containers were made of polypropylene (PP), they didn’t behave similarly. Compounds that were extracted from PP vials from different manufacturers were not always the same. Although the number of spectral types that are recorded is large, this article focuses on a few whose interpretation is interesting. The goal was to figure out when it makes sense to employ Raman microscopy for such identification. The selection of solvents for generating extractables and leachables from these polypropylene vials was informed by two USP publications (1,2). Polished stainless steel slides were used as substrates for the analysis because most metals, including stainless steel, do not have a Raman spectrum. These slides virtually provided a background-free substrate for the spectra. For each vial, samples were prepared immediately after receipt and then approximately 10 days after receipt. After the droplets dried, a mosaic micrograph was recorded with a low magnification objective. Then, the regions of interest were selected and imaged at 50x or 100× magnification before spectra were recorded. Interestingly, it was the 638-nm laser line that provided the best results; there was often fluorescence at 532 nm, the signal-to-noise (S/N) using the 785-nm laser was significantly poorer, and the sensitivity in the CH/NH region was compromised. Because of differences in solubility, if there are more than one species in a sample, they tend to separate during precipitation so spectra of the different species are recorded separately. In all cases, spectra were recorded from multiple spots with similar morphology to ensure that a spectrum was representative of the sample. Although multiple spectra can be recorded with the mapping function (that is, in a two-dimensional [2D] area with evenly spaced points), we more often used a function where we could select points in the image. By selecting spots with the same morphology, the analysis time was significantly reduced compared to what would have been required for a map acquisition. To improve the S/N of the spectra, identical multiple spectra from a given data set were averaged together.

We used KnowItAll (KIA) (3) software (Wiley) for spectral interpretation. To optimize the relative intensities in the spectra for matching, spectra were collected with the instrument correction spectrum (ICS) function turned on. If a suitable match did not appear, we used standard rules for spectral interpretation to provide an identification of at least the class of molecule represented by the spectrum.

Identification of Unknowns
To demonstrate the functionality of our method, Figure 1 shows the spectrum of one of the vials, as identified as polypropylene (PP) in KIA. However, you may notice that I have not chosen the spectrum with...
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the highest hit quality index (HQI). The first spectrum, with an HQI of 92.1, has extra bands near 1620 and 1650 cm\(^{-1}\) that are not in my spectrum. The second spectrum, with an HQI of 90.1, is identified as a copolymer of PP and polyacrylic acid (6%). For the moment, I am assuming that these tubes are pure PP, possibly containing some additives, so I have chosen the third entry. The ambiguity in even such a simple query indicates the reasons that some purist spectroscopists warn against solely using spectral data bases for identification.

### Results from Vials Exposed to Saline

Figure 2 shows mosaic images of deposits from centrifuge vials from the three vendors. Many of the deposits indicate the morphology of NaCl crystals, but with material of more disordered morphology adhering to the NaCl cubes. Of course, NaCl has no first-order Raman spectrum, so the spectra that we show were acquired from material clinging to the salt crystals. Figure 3 shows spectra of deposits from vials exposed to saline from each of the 3 suppliers, with the spectrum of PP shown at the bottom for easy reference. The starting observation is that each vial yielded different spectra. When a spectrum indicated the presence of elemental carbon, its two bands had been eliminated manually before plotting in Figure 3 or importing into the KIA software.

Each spectrum was examined separately in the KIA software, and the results are displayed in Figure 4. None of the matches are as good as that for PP, but there is ample information present. I should explain how I decide that a match is “good” when a match of the quality of the PP does not appear. The most important thing to understand is that the HQI represents the numerical overlap of the query spectrum with a spectrum from the data base. If there is a baseline, it will tend to overwhelm the HQI without really representing the species present. So the first thing to do is to subtract any baseline in your query spectrum and to enable baseline subtraction in KIA. I have also found that if there are broad bands in my spectrum, for instance from carbon, the searching algorithm finds carbon before anything else. Therefore, it is often helpful to remove the carbon contribution manually from the query spectrum. I will
be the first to admit that doing so is not rigorous, but it is effective. That is because looking for a mixture spectrum with sharp bands and the carbon spectrum is not always straightforward because the carbon spectrum is so variable.

So if a really good match does not pop up, the question is how to find the “best” match. What I do is to examine the listing in software, which is arranged in decreasing values for HQI while also examining the spectral pattern. I want to find a hit that has prominent bands in the same region as the prominent bands in the query spectrum. Unfortunately, this is not a simple selection of the spectrum with the highest HQI because of the reason explained in the previous paragraph.

So now let’s consider the results of the species found in the saline solutions from the three vendors’ vials. The first is a small molecule of 3-hydroxy butanoic acid. The second had two spectra—the first, a block copolymer of styrene isoprene, and the second, a spectrum of a dye, Sepisol Fast Blue. The spectrum of the deposit from the third vendor’s vial matched best to a mixture of poly (N-vinyl pyrollidone) and naphthalene 1,3,6 trisulfonic acid trisodium salt.

In Figure 4a, the match to 3-hydroxy butanoic acid is fairly good except there is no >C=O band in my spectrum at approximately 1750 cm\(^{-1}\). In fact, this spectrum had the presence of the broad carbon bands near 1340 and 1600 cm\(^{-1}\) that were interfering with my search so I eliminated them manually, and a small feature at ~1750 cm\(^{-1}\) may have been buried in the broad carbon band that I subtracted. Figure 4a is an example that illustrates the hazards of this kind of operation. In addition, my spectrum also shows a broad doublet above 3000 cm\(^{-1}\), which indicates the presence of residual water in the deposit.

Figure 4bi shows the best match to a copolymer of styrene isoprene, which was found in SearchIt but not IDExpert. In IDExpert, the sharp band at approximately 1000 cm\(^{-1}\) was never picked up, probably because it is sharp and at low intensity and would thus have a low contribution to the HQI. In addition, a sharp band near 1660 cm\(^{-1}\) was also missed. However, it is well known that many aromatics have a doublet at 1000–1040 cm\(^{-1}\) and a CH stretch near 3060 cm\(^{-1}\) and 1660 cm\(^{-1}\) often indicates the presence of olefinic >C=C<. Note that SearchIt found the copolymer of styrene isoprene on its first hit. In addition, the relative intensities of these bands at 1000 and 1660 cm\(^{-1}\) varies between my spectrum and that in the database, presumably because of the relative concentrations of the aromatic to olefinic species.

Figure 4bi shows the second spectrum observed in the deposit of this vial and identified it as Sepisol Fast Blue. It turns out that the vials from this vendor were colored, and a comparison of this spectrum in Figure 3bii to that of the colored vial (not shown), the spectrum of the colored vial matched a combination of that of PP and that of the spectrum of Sepisol Fast Blue.

Figure 4c shows a “best” match to the spectrum of the third vendor to a mixture of poly (N-vinyl pyrollidone) and naphthalene 1,3,6 trisulfonic acid trisodium salt. Although the match is not perfect, the prominent bands in the composite spectrum do overlap with the prominent bands in the query spectrum. Are my bands broadened by disorder in the polymer phase and interactions with the smaller molecule? It is hard to say, but it is certainly a possibility. This example is a case where liquid chromatography–mass spectrometry (LC–MS) or gas chromatography–MS (GC–MS) could be helpful in determining the origin of this contaminant.

**Why Are These Molecules Present in the PP vials?**

Additives are added to polymers for many reasons, which include antioxidant functionality, gas barrier, physical flexibility, and other reasons. The selection of the additive is dictated by the desired final properties of the material. I am not a polymer engineer so I cannot say what could be the reason for finding the products that we did in these saline solutions. However, in the future, after we have analyzed the deposits from all of the solutions, we may see a recognizable pattern.

**An Example Whose Origin is Clear**

In this article, there is not enough space to review and analyze the total data set. However, I want to show one example that illustrates the identification of a deposit whose presence I do understand. Figure 5 shows the result of a search in the KIA software of a spectrum deposited from a vial of the third vendor that had been exposed to the phosphate buffer at 100 °C. The match is excellent for a silicone oil. In fact, I have a spectrum of a solid silicone (not shown) whose spectral peaks match just

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- Fluorescence & Phosphorescence Lifetime Imaging (FLIM/PLIM)
as well, but maybe with different relative intensities. I suppose the difference between solid silicone and silicone oil could be simply the molecular weight, and we know that the Raman spectrum is not very sensitive to molecular weight. We also know that in a solid pellet that has presumably been extruded from the melt, there can be molecular orientation that can affect the relative intensities. Can we make sense of the presence of silicone oil in the deposit? Of course! It is often added as a release agent during a molding or extruding operation.

Summary

In an effort to evaluate the potential of Raman microscopy to identify extractables and leachables from polymers, I collected spectra from three sets of polypropylene centrifuge vials from three vendors exposed to 10 different solutions designed to tease out material hiding in the polymer matrix. I examined deposits, for the most part, only from saline solutions. I have described how I collected the spectra, and then how I prepared them for analysis in the KIA software. It is not always clear why particular molecules are being detected, but I picked one example where its presence as a release agent was clear.

The real question is, why bother with all of this? The standard analytical method for identifying extractables and leachables is liquid or gas chromatography combined with mass spectroscopy (LC–MS or GC–MS). What Raman can do that those standard techniques cannot is identify minute amounts of material—typically 1–2 µm × 1–5 µm deep. And there are no waste products from the analysis that need to be disposed of. Is the information the same? Maybe yes and maybe no. The measurement is done on intact material whereas MS tears the molecule apart. There may be cases where information is lost in tearing the molecule apart.

From my discussions with Mark Witkowski, I understand that the standard LC–MS and GC–MS techniques have difficulty identifying inorganic materials. In contrast, Raman spectroscopy is equally active for inorganic and organic materials.
compounds. In my column last November, where I discussed spectral identification, I showed the excellent identification of a particle of WO$_3$ (4).

For the polymer engineer who is selecting which additives to put in her product, a Raman microscope measurement could be an easy way to determine the safety of the selected additive.

References
(3) KnowItAll, Wiley.
(4) F. Adar, Spectroscopy 36(11), 8–13 (2021).
Expanding the Applicability of Handheld Raman Spectroscopy

Metrohm develops Raman instruments and techniques to expand the applicability of spectroscopy for scientists, instrument developers, and clients.

Advances in chemical and compound analysis utilizing robot integration, fluorescence mitigation, and techniques like SERS (surface-enhanced Raman scattering) are improving the utility of Raman spectroscopy. To delve deeper into this topic, Spectroscopy sat down with Dr. Adam J. Hopkins [Spectroscopy Product Manager, Metrohm USA] and Dr. Keith Carron [CEO, Metrohm Raman] to discuss the changing market of Raman technology.

SPECTROSCOPY: Dr. Carron, you’ve been developing miniature Raman instruments for about 20 years, starting with the very first handheld at DeltaNu. In that time, how has the market for handheld Raman changed?

CARRON: I think what has changed is our understanding, as scientists and instrument developers, as to what the customer needs. We began thinking about handheld Raman after 9/11, and there is a requirement for field instruments versus taking samples to the lab. Our thoughts were really, at first, Star Trek tricorder-type devices. The way we decided to do that was to build a small device, load thousands of spectra of known materials, point it at something, and tell you what it is. That’s still the goal, but what we know now is that simply loading thousands of compounds of chemical names and spectra doesn’t produce a very meaningful real-world result. What people encounter in the real world are mixtures, maybe trace compounds, and they often have interferences from materials that fluoresce.

SPECTROSCOPY: Mixtures, trace components, and fluorescence—how do Raman instruments handle these?

CARRON: With mixtures, we ask if the end user cares about decomposing a mixture; if not, then we treat mixtures as a pure material. We do a correlation, matching to a library, and we report the primary material. If they care about what a mixture contains—for example, cocaine cut with caffeine and baking soda—then we have algorithms that we’ve developed that decompose the total Raman spectrum into components and identify the most prominent ones to the user.

HOPKINS: The other side of mixtures is something that we see as having a big impact on handheld measurements - inhomogeneity. Many times, when we make a Raman measurement, we have a very small spot size: 100 to 200 microns in diameter. [This] is so small that if you point your sensor at two different locations on a sample, there’s a good chance you’re going to get a different result, because the instrument sees only, say, a grain of material. If we’re talking about packaging, we encounter a crease in the packaging material versus an area that’s flat. Keith’s team at Metrohm Raman developed Orbital Raster Scan technology to overcome this problem. They developed it for surface-enhanced Raman spectroscopy, also known as SERS, which we’ve been applying to both that SERS for trace measurement, but also into bulk measurements.

SPECTROSCOPY: That leads us to trace components. How are Metrohm Raman’s instruments handling trace analysis?

CARRON: My original work in Raman spectroscopy, going all the way back to 1980, was related
to a special method called SERS; Adam mentioned that. SERS stands for surface-enhanced Raman scattering. SERS is a nanoparticle technique. It's often misunderstood as a way to enhance the signal from everything in a sample. People at first thought it was a miracle. You sprinkle magic nanoparticle dust on your sample and suddenly you see trace materials. That's not exactly the case. SERS enhances a small class of materials that happen to include, fortunately, most illicit drugs, food contaminants, usually materials that are hazardous to humans. It does not enhance all the materials in the sample. It really only enhances those that bind to the nanoparticles. What this does is it permits SERS to act as a separation technique, where what you don't want to see is not enhanced and what you do want to see, what is actually sticking to the nanoparticles, is enhanced. The enhancement is as much as one million or 10 millionfold.

SPECTROSCOPY: Before moving to fluorescence, are there differences in the libraries for SERS compared to normal Raman identification?

CARRON: Yes. This stems from fundamental differences between SERS and normal Raman, as I described previously. The SERS spectra come from molecules that have absorbed chemically to the nanoparticles, and this provides or creates a shift in some of the Raman bands. We really can't take the bulk Raman spectrum of chemicals that we collect and expect it to match to a SERS library. What we do in the case of a SERS library is we actually do something like a barcode where we look for positions of bands. If the bands are there, then we state that the material is there.

SPECTROSCOPY: That brings us to fluorescence. There are a lot of approaches to overcoming fluorescence. How are your Raman instruments handling this?

HOPKINS: The way most people think to overcome fluorescence is by changing the laser wavelength, either moving down into the deep ultraviolet, or up into the near infrared. The former, moving down into the ultraviolet, isn't feasible for handheld systems. Moving up into the near infrared, say, using 1064 nanometer Raman, results in a less sensitive instrument. That creates challenges in the chemical and security and defense industries, where many materials are highly reactive. The higher laser powers and longer exposure times needed to make a measurement conflict with the need for safety. To meet those requirements, Metrohm Raman developed XTR technology to bring the fluorescence reduction capability of 1064 nanometer Raman to 785.

SPECTROSCOPY: What is XTR and how does it make handheld Raman safer for the chemical and other industries?

CARRON: XTR is a technique. The term XTR comes from the word extraction and it's a three-letter acronym for eXTRaction. What we're doing is we're extracting the Raman signal from the fluorescent background. It's a highly mathematical technique. It's patent pending at this moment. What we do is we take the total signal that the instrument sees, which includes fluorescence and Raman, and the fluorescence is interfering with the Raman spectrum. We actually separate these into two spectra, or two vectors, in mathematical talk. One of those spectra is the pure fluorescence, and one spectrum is the pure Raman spectrum. What we do then with the MIRA XTR is we only use the pure Raman spectrum without any associated fluorescence or any interferences that would be there. What this means is that, in the XTR, we don't have artifacts associated with traditional methods that are used. Baseline methods, such as curve fitting derivatives, filtering methods—we've removed all of those and we really create only a pure Raman spectrum.

HOPKINS: The only thing I want to point out is that we're able to take that XTR technology and give it to the chemical and petrochemical industries which have a lot of highly fluorescent materials that are dangerous to handle. We've added standoff Raman capability to our MIRA XTR. With this capability, an operator can look through a reactor or pipeline sight glass, or down into a chemical drum or even a rail car, take a Raman spectrum, and identify the materials without sampling. This is a major safety improvement.

SPECTROSCOPY: Finally, we've seen a lot of buzz over the past few months about robot integration with the MIRA. Can you comment on this?

CARRON: First, let me say why we want to integrate with a robot. That is so that we can perform what's called Sensitive Site Exploration (SSE). The goal is to avoid putting humans at risk in sites where there might be hazardous chemicals or explosive potentials and send in a robot. We partnered with Boston Dynamics to integrate the MIRA XTR with a standoff Raman capability to put on their Spot robot platform. We've added to this integration of Raman, the whole sensor package, so that we can also identify combustible gases, radiological hazards, air quality risks, so on. The robot really is carrying a complete package to detect hazards and to have a Raman system to identify hazards that have been detected. This is our commitment to improving Raman analysis of hazardous situations.

Metrohm is a world-renowned manufacturer of high-precision instruments for chemical analysis. For more information, please visit metrohm.com.
We continue our survey of the spectra of carbonyl-containing polymers by looking at the spectrum of cellulose acetate. What makes cellulose acetate unique is that it is a carbohydrate molecule that is reacted to obtain pendant ester groups. I will also introduce you to polycarbonates. Carbonates are a carbonyl-containing functional group that contain three oxygen atoms. An example of an economically important polycarbonate is Lexan, which is made into windows and car parts. In this column, we examine its spectrum in detail.

I stated in my last column (1) that a polyester is a polymer with an ester group in its backbone. But what about polymers with pendant ester groups? What do we call those, and where should we discuss them? For lack of a better term, I will call polymers with pendant ester groups pendant ester polymers (PEPs). A common PEP is the family of cellulose acetates. These polymers are made when a polymer, cellulose, reacts with acetic acid. Figure 1 shows the synthesis of cellulose diacetate.

Acetic anhydride is sometimes used instead of, or in addition to, acetic acid (2). Given that paper is made from cellulose and acetic acid is found in vinegar, you could in theory make cellulose acetate at home, but I wouldn’t recommend it because you typically need a sulfuric acid catalyst. The cellulose monomer has three O-H groups that can react to form an ester. Thus, cellulose acetate, cellulose diacetate, and cellulose triacetate are possible. Cellulose acetate is commonly found in consumer products, including cigarette filters and playing cards.

We have previously discussed the infrared (IR) spectrum of cellulose (3), and we have also discussed the spectra of esters (4) and polyesters (1). Recall that acetate esters have a special high wavenumber C-C-O stretching peak at ~1240 cm⁻¹ (going forward, assume all peak positions are in cm⁻¹ even if not so expressed) caused by a mass effect (5). Normally saturated esters, like those in cellulose acetate, exhibit C-C-O stretches between 1210–1150 cm⁻¹ (4). Therefore, the acetate C-C-O peak at 1240 cm⁻¹ breaks one of our rules, but it is a useful rule break because it is one we understand and can make use of. Acetate esters are common in the world of polymers and even in the world of controlled substances; for example, heroin contains this functional group. Thus, given the importance of acetate esters, it is just as well they contain a special peak signifying their presence in a sample.

Figure 2 shows the structure of cellulose triacetate and the IR spectra of cellulose acetate and cellulose triacetate. Note that the alcohol O-H stretch at 3484 is bigger in cellulose acetate than in the triacetate because in the triacetate more of the O-H groups have reacted to form esters. Otherwise, this spectrum contains the classic saturated ester Rule of Three peaks (4) with the C=O stretch at 1748 cm⁻¹, the acetate ester C-C-O stretch at 1237 cm⁻¹, and the O-C-C stretch at 1051 cm⁻¹.

Organic Carbonates Review

Organic carbonates are a functional group similar to esters, so it is appropriate to group polycarbonates with PEPs.
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The chemical term carbonate is a little confusing. In general, the term refers to a functional group with the formula \( \text{CO}_3^{2-} \). There exist inorganic carbonates that contain the \( \text{CO}_3^{2-} \) ion where each carbon-oxygen bond has the same bond order (6).

Although this functional group contains a carbon atom, it acts inorganic because it forms ionic bonds and comprises rocks such as limestone. The literature provides more information on the spectra of inorganic carbonates (6). We will discuss the spectra of inorganic carbonates here soon when we cover inorganic molecules.

Organic carbonates contain a carbon atom with three oxygens bonded to it, but the bonding is covalent and consists of C=O and C-O bonds, which is shown in Figure 3.

Note that organic carbonates contain two alpha carbons. If both alpha carbons are saturated, the carbonate is saturated. If one alpha carbon is aromatic and one is saturated, the carbonate is said to be mixed. If both alpha carbons are aromatic, the carbonate is aromatic.

As you can see in Figure 3, carbonates are symmetrical, and each half can be thought of as an ester, with each half having a carbonyl carbon, ester oxygen, and an alpha carbon. Note that the carbonyl carbon has not one oxygen attached to it as in an ester but two, which means that there are two ester oxygens and two alpha carbons as seen.

The IR Spectra of Organic Carbonates

Given the structural similarity between esters and organic carbonates we might expect carbonates to follow the Rule of Three as esters do. Carbonates do have three intense peaks like an ester (7), but the vibrations responsible are a little different than in esters because the structures of esters and carbonates are different. Briefly, esters have a C=O stretch around 1700, a C-C-O stretch near 1200 cm\(^{-1}\), and an O-C-C stretch around 1100 cm\(^{-1}\). Carbonates have C=O and O-C-C stretches, but unlike esters have an O-C-O linkage and hence an O-C-O asymmetric stretching peak instead of a C-C-O peak.

Table I shows the group wavenumbers for the three varieties of organic carbonates.

Note that the C=O stretch is different for all three types of carbonates, and that for mixed and aromatic carbonates particularly the C=O stretch is much higher than any ester C=O stretch we have studied, making these two types of organic carbonate easy to spot. Table I also shows that the organic carbonate O-C-O stretching peak position goes down as we move from the saturated, mixed, and aromatic versions of the functional group.

The chemical term carbonate is a little confusing. In general, the term refers to a functional group with the formula \( \text{CO}_3^{2-} \). There exist inorganic carbonates that contain the \( \text{CO}_3^{2-} \) ion where each carbon-oxygen bond has the same bond order (6).

Although this functional group contains a carbon atom, it acts inorganic because it forms ionic bonds and comprises rocks such as limestone. The literature provides more information on the spectra of inorganic carbonates (6). We will discuss the spectra of inorganic carbonates here soon when we cover inorganic molecules.

Organic carbonates contain a carbon atom with three oxygens bonded to it, but the bonding is covalent and consists of C=O and C-O bonds, which is shown in Figure 3.

Note that organic carbonates contain two alpha carbons. If both alpha carbons are saturated, the carbonate is saturated. If one alpha carbon is aromatic and one is saturated, the carbonate is said to be mixed. If both alpha carbons are aromatic, the carbonate is aromatic.

As you can see in Figure 3, carbonates are symmetrical, and each half can be thought of as an ester, with each half having a carbonyl carbon, ester oxygen, and an alpha carbon. Note that the carbonyl carbon has not one oxygen attached to it as in an ester but two, which means that there are two ester oxygens and two alpha carbons as seen.

The IR Spectra of Organic Carbonates

Given the structural similarity between esters and organic carbonates we might expect carbonates to follow the Rule of Three as esters do. Carbonates do have three intense peaks like an ester (7), but the vibrations responsible are a little different than in esters because the structures of esters and carbonates are different. Briefly, esters have a C=O stretch around 1700, a C-C-O stretch near 1200 cm\(^{-1}\), and an O-C-C stretch around 1100 cm\(^{-1}\). Carbonates have C=O and O-C-C stretches, but unlike esters have an O-C-O linkage and hence an O-C-O asymmetric stretching peak instead of a C-C-O peak.

Table I shows the group wavenumbers for the three varieties of organic carbonates.

Note that the C=O stretch is different for all three types of carbonates, and that for mixed and aromatic carbonates particularly the C=O stretch is much higher than any ester C=O stretch we have studied, making these two types of organic carbonate easy to spot. Table I also shows that the organic carbonate O-C-O stretching peak position goes down as we move from the saturated, mixed, and aromatic versions of the functional group. The O-C-C
stirring peak range is the same for all three types of carbonates. The saturated carbonate C=O stretch falls in the same range as that of saturated esters (4). However, saturated carbonates have their O-C-O peak from 1280 to 1240 cm\(^{-1}\), whereas saturated esters have their C-C-O peak lower from 1210 to 1160 cm\(^{-1}\). It is the relative position of these two peaks that allows one to distinguish saturated esters and carbonates from each other.

The IR spectrum of an aromatic carbonate and a common polycarbonate, Lexan (poly 2,2-Bis[4-hydroxyphenyl]propane), is seen in Figure 4.

Lexan is an aromatic carbonate because the two alpha carbons are part of benzene rings. The peak labeled A at 1777 cm\(^{-1}\) is undoubtedly a C=O stretch based on its strength and position. The carbonyl stretch of aromatic carbonates in general falls from 1820 to 1775 cm\(^{-1}\). The C=O stretch of mixed carbonates falls from 1790 to 1760 cm\(^{-1}\), and for saturated carbonates, this peak is seen at 1740±10. In Figure 4, the O-C-O stretch is labeled B at 1230 cm\(^{-1}\). For aromatic carbonates, this peak is typically found from 1230 to 1205 cm\(^{-1}\), whereas for mixed carbonates, it falls between 1250–1210 cm\(^{-1}\), and for saturated carbonates, it falls from 1280 to 1240 cm\(^{-1}\). The O-C-C stretch in Figure 4 is at 1015 cm\(^{-1}\), and for all carbonates, this peak falls from 1060 to 1000 cm\(^{-1}\).

Figure 5 shows the spectrum of a mixture of polystyrene and Lexan.

We have studied the spectrum of polystyrene previously (8). In Figure 5, we can see C-H stretches above 3000 cm\(^{-1}\) from the aromatic rings in both Lexan and polystyrene, aromatic ring modes at 1601 cm\(^{-1}\) and 1493 cm\(^{-1}\), the ring bend at 698 cm\(^{-1}\), and the C-H wag at 757 cm\(^{-1}\) from the mono-substituted benzene ring in polystyrene (8). Note that the 698 cm\(^{-1}\) peak is the biggest one in this spectrum. The Lexan peaks are the C=O stretch at 1774 cm\(^{-1}\) labeled A, the O-C-O stretch at 1227 cm\(^{-1}\) labeled B, and the O-C-C stretch at 1015 cm\(^{-1}\) labeled C. These peaks are close to their positions in pure Lexan.

Figure 6 shows the spectrum of a mixture of Lexan and polybutylene terephthalate. We saw the spectrum of pure polybutylene terephthalate (PBT) in the last column (1).

The three main peaks from the polycarbonate Lexan are present, with the C=O stretch falling at 1777 cm\(^{-1}\), the O-C-O stretch at 1230 cm\(^{-1}\), and the O-C-C stretch at 1015 cm\(^{-1}\). The “Rule of 3” peaks are present for PBT with the C=O stretch at 1719 cm\(^{-1}\), the C-C-O at 1280 cm\(^{-1}\), and the O-C-C stretch at 1118 cm\(^{-1}\). As a result of these being carbonate and ester functional groups present, there are two carbonyl stretches. Also, because both these functional groups have multiple C-O stretching vibrations, there are eight peaks between 1300–1000 cm\(^{-1}\). The two Lexan peaks in this region were easy to spot, but the PBT peaks at 1280 and 1118 cm\(^{-1}\) are barely discernible as shoulders, and I only found them after examining an expanded view of the spectrum. This observation points out one of the problems with mixtures, which is the fact that peaks from one molecule can hide the peaks of other molecules. We have discussed techniques for getting around the mixture analysis problem in previous columns, including spectral subtraction (9) and library searching (10).
Colorimetric Discrimination of Pd$^{2+}$ and Hg$^{2+}$ Ions in Solvent and Solid-Film State Using Organic Acid-Assisted Green Synthesized Silver Nanoparticles

Kaiyu Zhang, Yuxin Sang, Qinxing Sun, and Weina Li

In this study, a colorimetric discrimination of Pd$^{2+}$ and Hg$^{2+}$ ions in the solvent and solid film states in a silver nanoparticle (AgNP) sensing system is presented. First, silver nanoparticles were prepared by reducing AgNO$_3$ with sodium borohydride in the presence of chitosan and different organic acids, including acetic acid, propanedioic acid, and citric acid. The addition of different organic acids allowed for the surface plasmon resonance (SPR) intensity and size distribution of the AgNPs to be adjusted. Chitosan acts as a stabilizer and complexing agent, endowing AgNPs with excellent film-forming properties. Then, the chitosan-stabilized AgNPs in the solvent and solid-film state are used to detect metal ions. In the presence of Hg$^{2+}$ and Pd$^{2+}$ ions, the color of the AgNP solution changed rapidly from pale yellow to colorless and light brown, respectively. The characteristic SPR peaks of the AgNPs also disappeared completely, and the solid films of AgNPs with a yellowish-brown color also changed rapidly to colorless and dark brown with the addition of Hg$^{2+}$ and Pd$^{2+}$ ions, respectively. The discrimination of Hg$^{2+}$ and Pd$^{2+}$ ions can be clearly observed in both the solvent and the solid film state. However, the addition of other metal ions cannot change the color of the AgNPs.

With the rapid expansion of industry, global environmental pollution is becoming more serious. Heavy-metal ion contamination is one of the most concerning types of environmental pollution. These contaminants can cause acute or chronic toxicities to the human body, leading to various diseases (1). For example, palladium has the propensity to bind to deoxyribonucleic acid (DNA), thiol-containing amino acids, proteins, and other biomolecules, which disturbs some cellular processes and causes serious physiological disorders (2,3). Mercury exposure can lead to severe damage of the central nervous and endocrine systems, resulting in detrimental effects on several important organs, such as the brain and kidneys (4,5). Thus, the fast and convenient monitoring of palladium and mercury is important for waste management, environmental protection, and public health. Conventional analytical methods for palladium and mercury detection include atomic absorption spectroscopy (AAS) and atomic emission spectroscopy (AES) (6,7), solid-phase microextraction–high performance liquid chromatography (SPME–HPLC) (8,9), inductively coupled plasma–mass spectrometry (ICP-MS) (10,11), ICP–atomic emission spectroscopy (ICP-AES) (12,13), electrochemistry (14,15), and adsorption dissolution voltammetry (16,17). These instrumental techniques can provide direct and quantitative information about palladium and mercury concentrations, but these techniques are time-consuming, costly, and not well-suited for the quick detection of palladium and mercury in the field. Fluorimetric and colorimetric methods provide a useful alternative for the detection of mercury and palladium because of their relative simplicity, cost-effectiveness, and nondestructive nature (18). Fluorescent sensors for Hg$^{2+}$ and Pd$^{2+}$ ions reported are mainly based on the coordination mechanism of organic probes with Hg$^{2+}$ and Pd$^{2+}$ ions (19–21), in which the fluorescence signals of the probes are always quenched because of the efficient spin-orbit coupling and non-radiation deactivation of the excited states of Hg$^{2+}$ and Pd$^{2+}$ ions (22–24). However, they suffer from different degrees of interference with other transition metal ions, and most of these sensing systems possess disadvantages, such as requiring high synthetic expertise to prepare multistep...
and expensive fluorescence probes and laborious purification steps.

Colorimetric methods based on the noble metal nanoparticles, which involve the naked-eye detection of a change in color caused by the distance-dependent surface plasma resonance (SPR) phenomena, have been developed for various heavy metal ions (25). For the detection of Hg\(^{2+}\) ions, most of the colorimetric sensors are based on AuNPs (26). The interaction between AuNPs and Hg\(^{2+}\) ions results in the aggregation of AuNPs with the color change from red to an aggregation-induced purple or colorless (27,28) or the anti-aggregation of AuNPs with a color change from pink to colorless (29). Although AuNPs as colorimetric sensors are promising tools for the detection of Hg\(^{2+}\), they usually require careful modification of AuNPs with DNA or thiol-containing organic molecules under precise experimental conditions, which makes them time-consuming and costly. Compared with AuNPs, AgNPs can also be Hg\(^{2+}\) colorimetric sensors, which are mostly based on the redox reaction between AgNPs and Hg\(^{2+}\) (30–32) with a color change from yellow to colorless. For colorimetric sensing of Pd\(^{2+}\) ions, Anwar and coworkers reported cationic pyrazinium thioacetate-stabilized AuNPs serving as an effective Pd\(^{2+}\) ion naked-eye sensor with color changing from pink to colorless (33). However, AgNPs have never been exploited as Pd\(^{2+}\) colorimetric sensors (34). Moreover, the colorimetric sensing of Pd\(^{2+}\) and Hg\(^{2+}\) ions in one noble metal nanoparticles sensing system has never been realized (35).

In this study, we presented a colorimetric discrimination of Pd\(^{2+}\) and Hg\(^{2+}\) ions in one AgNP sensing system for the first time. By introducing the biopolymer chitosan as the stabilizer and complexing agent, this system was able to distinguish Pd\(^{2+}\) and Hg\(^{2+}\) ions simultaneously in the solvent and solid-film state. First, silver nanoparticles were prepared by reducing AgNO\(_3\) with sodium borohydride in the presence of chitosan and different organic acids, including acetic acid (AA), propane-dioic acid (PA), and citric acid (CA). It was demonstrated that the addition of different organic acids could finely adjust the SPR intensity and size distribution of AgNPs. This study also revealed for the first time the effect of organic acid in the synthetic procedure of AgNPs. Chitosan, which is a biocompatible polysaccharide with largely amount of free amino and hydroxyl groups exhibiting unique polycationic, chelating, and film-forming properties, acted as a stabilizer and complexing agent, leading to the formation of composite solid films (36). Then, the chitosan-stabilized AgNPs in the solvent and solid-film states

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were used to detect metal ions. In the presence of Hg$^{2+}$ and Pd$^{2+}$ ions, the color of the AgNP solution changes rapidly from pale yellow to colorless and light brown, respectively. Correspondingly, the characteristic SPR peaks of the AgNPs completely disappeared. The solid film of AgNPs with its yellowish-brown color also changed rapidly to colorless and dark brown with the addition of the Hg$^{2+}$ and Pd$^{2+}$ ions, respectively. The discrimination of Hg$^{2+}$ and Pd$^{2+}$ ions was clearly observed in both the solvent and the solid-film state. However, the addition of other metal ions did not change the color the AgNPs. It was further revealed that this method showed a linear response range of 50–90 μm and 100–300 μm for Hg$^{2+}$ and Pd$^{2+}$. The limit of detection (LOD) was estimated to be $2.26 \times 10^{-7}$ M and $1.05 \times 10^{-6}$ M for Hg$^{2+}$ and Pd$^{2+}$, respectively. The colorimetric discrimination of the Hg$^{2+}$ and Pd$^{2+}$ ions in solvent and solid film provided a new avenue for simultaneous on-site detection metal ions by the naked eye.

Results and Discussion
Preparation of AgNPs
Colloidal silver nanoparticles were prepared by reducing AgNO$_3$ using sodium borohydride with chitosan as the stabilizer and complexing agent in the presence of different kinds of organic acids (AA, PA, or CA) at room temperature, and the resulting solutions were labeled as AgAA-CHIT, AgPA-CHIT, and AgCA-CHIT, respectively. The first optical indication of AgNP formation was provided by the color change of the solution from colorless to pale yellow, and it was further monitored by UV-vis spectroscopy. As shown in Figure 1, the absorbance intensity follows the order of AgPA-CHIT > AgCA-CHIT > AgAA-CHIT, suggesting that these organic acids participate in the reaction, and the reduction rate of Ag$^+$ to Ag$^0$ is strongly affected by the nature of the organic acid (37).
When preparing the three organic acid solution with the same concentration (0.20 mol/L), the pH values were 1.90, 2.26, and 3.01 for PA, CA, and AA, respectively, implying that a pH effect cannot be ruled out in the formation of AgNPs. PA-CHIT with a lower pH and a higher degree of protonation of amino groups of chitosan helped promote the reduction of the silver precursor (38), leading to a higher absorption intensity.

As displayed in Figure 1, the formation of metallic AgNPs in the AgAA-CHIT and AgCA-CHIT solutions was confirmed by the appearance of the SPR band at 404 nm with the similar intensity in the corresponding UV-vis spectra. According to the SPR peak position and intensity, it was estimated that the average diameter of the AgNPs was 27 nm (39) for both samples (Table II). When the AgNPs were synthesized in the chitosan-propanedioic acid solution, different behavior was observed. The SPR band showed a slight blue shift to 398 nm, and the absorption intensity displayed significant enhancement (Figure 1), which is indicative of the smaller and higher concentration of metal nanoparticles. The size and morphology of AgNPs were estimated by transmission electron microscopy (TEM) and are displayed in Figure 2a, which shows the presence of polydispersed spherical nanoparticles in the size range of 11–18 nm. Compared with AgAA-CHIT and AgCA-CHIT (Figure 2b–2c), AgPA-CHIT particles (Figure 2a) have better dispersion, particle size uniformity, and homogeneous morphology.

### Interaction of Silver Nanoparticles with Various Metal Ions

Because the silver nanoparticles synthesized in the presence of propanedioic acid have better dispersion, particle size uniformity, and absorption intensity, AgPA-CHIT particles were chosen to evaluate the response to various metal ions. The UV-vis absorption spectra and color change of AgPA-CHIT were taken in the presence of different metal ions, including Al\(^{3+}\), Mg\(^{2+}\), Cd\(^{2+}\), Zn\(^{2+}\), Co\(^{2+}\), Ni\(^{2+}\), Mn\(^{2+}\), Cu\(^{2+}\), Pd\(^{2+}\), and Hg\(^{2+}\). Figure 3 shows the effect of various metal ions on the freshly prepared AgPA-CHIT particles. The solutions in contact with Hg\(^{2+}\) and Pd\(^{2+}\) changed from pale yellow to colorless and light brown, respectively (Figure 3a), and the corresponding SPR band completely disappeared (Figure 3b). However, the effect of other metal ions on the color and SPR band of AgPA-CHIT particles was negligible. The color difference of AgPA-CHIT with Hg\(^{2+}\) and Pd\(^{2+}\) provided a method to visibly detect these two metal ions simultaneously with the naked eye. Moreover, the introduction of the bio-

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polymer chitosan as the stabilizer and complexing agent endowed the AgNPs with good film-forming properties. Therefore, the AgPA-CHIT film was further prepared to evaluate the metal selectivity. As shown in Figure 3c, when different metal ions with the concentration of $10^{-3}$ M were added to the AgPA-CHIT films, only the films contacting with the Hg$^{2+}$ and Pd$^{2+}$ ions were significantly different with the color changing from yellowish brown to colorless and brownish-black, respectively (the visualization images are taken on white paper, so the colorless film looks white). Color changes in the state of solution and film can be observed within one minute. The results revealed that discrimination of the Hg$^{2+}$ and Pd$^{2+}$ ions can be clearly observed in both the solvent and the solid-film state. Thus, it is suggested that the AgPA-CHIT particles with significant Hg$^{2+}$ and Pd$^{2+}$ differentiation properties could serve as a fast, simple, and convenient onsite naked-eye probe for Hg$^{2+}$ and Pd$^{2+}$ ions recognition.

Sensitivity and UV-vis Titration of Hg$^{2+}$ and Pd$^{2+}$ Ions

To further investigate the recognition mechanism of AgPA-CHIT to the Hg$^{2+}$ and Pd$^{2+}$ ions, the UV-vis titration and TEM images were further tested. As shown in Figure 4 and 5, the characteristic SPR band of AgPA-CHIT was observed at 398 nm, and the color of the solution is pale yellow in the absence of Hg$^{2+}$ and Pd$^{2+}$. Increasing the concentration of Hg$^{2+}$ to AgPA-CHIT, the color of the solution decreased, accompanying with the blue shifting and broadening of the SPR band. Finally, the solution turned colorless after the addition of 400 µM of Hg$^{2+}$ and the SPR band almost completely disappeared. When different concentrations of Pd$^{2+}$ to AgPA-CHIT was added, the color of the solution deepened gradually, accompanying the broadening and red shifting of the SPR band and finally turning to light brown after the ad-
dition of 400 μm of Pd$^{2+}$ and the SPR band almost completely disappeared.

To obtain further information about the characteristic of AgPA-CHIT in the absence and presence of Hg$^{2+}$ and Pd$^{2+}$, the samples were analyzed using TEM. The corresponding TEM images are displayed in Figures 2a and 6. It can be seen that well dispersed silver nanoparticles are presented in Figure 2a. After the addition of Hg$^{2+}$ to the AgPA-CHIT solution, the nanoparticles completely disappeared, which might be because of the redox reaction between Hg$^{2+}$ and zero-valent silver with the standard potential of 0.85 V (Hg$^{2+}$/Hg) and 0.8 V (Ag$^+$/Ag), respectively (40). It was proposed that after the addition of Hg$^{2+}$ ions to the freshly prepared AgPA-CHIT, mercury (II) ions bound to the surface of AgPA-CHIT particles to move the biological stabilizer chitosan away from the silver surface, leading to a redox reaction between the silver and mercury ions (Scheme 1). This redox reaction may account for the blue shift of the SPR band of AgNPs. The addition of Pd$^{2+}$ to the AgPA-CHIT solution caused the nanoparticles agglomerated to form larger ones (Scheme 1), which was also in accordance with the red shift of the SPR bands.

The limit of detection (LOD) for the Hg$^{2+}$ and Pd$^{2+}$ ions was further determined by using the characteristic SPR peak of AgPA-CHIT. Three repeated experiments demonstrated that the concentration of both metal ions <10 μm did not change the color of AgPA-CHIT. As shown in Figure 4b and 5b, the absorption peaks of AgPA-CHIT decreased by increasing the concentration of the Hg$^{2+}$ and Pd$^{2+}$ ions. There is a linear relationship between the absorption intensity changes and the linear response concentration ranges, which are 50–90 μm and 100–300 μm for Hg$^{2+}$ and Pd$^{2+}$, respectively. Thus, it was calculated that the AgPA-CHIT could be used for the colorimetric detection of Hg$^{2+}$ and Pd$^{2+}$ with the LODs at 2.26 × 10$^{-7}$ M and 1.05 × 10$^{-6}$ M, respectively (Figure 7). Compared with other sensors and methods for sensing of Hg$^{2+}$ or Pd$^{2+}$ (Tables III and IV), our proposed methods required neither careful modification of AgNPs nor a high cost of instrumentation. Moreover, the simultaneous discrimination of Hg$^{2+}$ or Pd$^{2+}$ has never been realized by the reported methods. The above results proved that chitosan-stabilized AgPA-CHIT can serve as a fast, simple, and convenient onsite naked-eye probe for Hg$^{2+}$ and Pd$^{2+}$ ions.

**SCHEME 1:** Proposed mechanism for AgPA-CHIT to discriminate Hg$^{2+}$ and Pd$^{2+}$ ions.

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**TABLE I: Recoveries of the AgPA-CHIT for the determination of Hg$^{2+}$ and Pd$^{2+}$ in drinking water and lake water samples ($n = 4$)**

<table>
<thead>
<tr>
<th>Samples</th>
<th>Spiked Hg$^{2+}$(µM)</th>
<th>Found Hg$^{2+}$(µM)</th>
<th>Recovery (%)</th>
<th>RSD (%)</th>
<th>Spiked Pd$^{2+}$(µM)</th>
<th>Found Pd$^{2+}$(µM)</th>
<th>Recovery (%)</th>
<th>RSD (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Drinking water</td>
<td>0</td>
<td>nd$^a$</td>
<td>-</td>
<td>-</td>
<td>0</td>
<td>nd</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td></td>
<td>50</td>
<td>48.4</td>
<td>96.8</td>
<td>2.20</td>
<td>100</td>
<td>101.3</td>
<td>101.3</td>
<td>1.12</td>
</tr>
<tr>
<td></td>
<td>70</td>
<td>70.6</td>
<td>100.9</td>
<td>1.08</td>
<td>200</td>
<td>182.5</td>
<td>91.3</td>
<td>0.88</td>
</tr>
<tr>
<td></td>
<td>90</td>
<td>87.2</td>
<td>96.9</td>
<td>0.95</td>
<td>300</td>
<td>292.7</td>
<td>97.6</td>
<td>1.43</td>
</tr>
<tr>
<td>Lake water</td>
<td>0</td>
<td>nd</td>
<td>-</td>
<td>-</td>
<td>0</td>
<td>nd</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td></td>
<td>50</td>
<td>49.2</td>
<td>98.4</td>
<td>1.24</td>
<td>100</td>
<td>98.0</td>
<td>98.0</td>
<td>1.21</td>
</tr>
<tr>
<td></td>
<td>70</td>
<td>69.3</td>
<td>99.0</td>
<td>1.22</td>
<td>200</td>
<td>195.8</td>
<td>97.9</td>
<td>0.97</td>
</tr>
<tr>
<td></td>
<td>90</td>
<td>88.1</td>
<td>97.9</td>
<td>1.85</td>
<td>300</td>
<td>291.6</td>
<td>97.2</td>
<td>1.65</td>
</tr>
</tbody>
</table>

*Source: $^a$ nd: not detected.

**TABLE II: pH value of the synthesis of AgNPs, the maximum absorbance of AgNPs, and particle size estimated from UV-vis spectra**

<table>
<thead>
<tr>
<th>Sample</th>
<th>pH</th>
<th>$\lambda_{\text{max}}$ (nm)</th>
<th>Average particle size (nm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>AgAA-CHIT</td>
<td>3.01</td>
<td>404</td>
<td>27</td>
</tr>
<tr>
<td>AgCA-CHIT</td>
<td>2.26</td>
<td>404</td>
<td>27</td>
</tr>
<tr>
<td>AgPA-CHIT</td>
<td>1.90</td>
<td>398</td>
<td>16</td>
</tr>
</tbody>
</table>

**TABLE III: Comparison of performance of different sensors for detecting Hg$^{2+}$**

<table>
<thead>
<tr>
<th>Sensors</th>
<th>LOD</th>
<th>Linear range</th>
<th>Reference</th>
</tr>
</thead>
<tbody>
<tr>
<td>Tween 20-AuNPs</td>
<td>100 nM</td>
<td>200–800 nM</td>
<td>(1)</td>
</tr>
<tr>
<td>Cit-AgNPs</td>
<td>50 nM</td>
<td>0–1000 nM</td>
<td>(2)</td>
</tr>
<tr>
<td>CP-AgNPs</td>
<td>4.125 µM</td>
<td>5–500 µM</td>
<td>(3)</td>
</tr>
<tr>
<td>AgNPs</td>
<td>8 nM</td>
<td>20–100 nM</td>
<td>(4)</td>
</tr>
<tr>
<td>AgPA-CHIT</td>
<td>$2.26 \times 10^{-7}$ M</td>
<td>50–90 µM</td>
<td>This work</td>
</tr>
</tbody>
</table>

**TABLE IV: Comparison of performance of different methods for detecting Pd$^{2+}$**

<table>
<thead>
<tr>
<th>Sensors</th>
<th>LOD</th>
<th>Linear range</th>
<th>Reference</th>
</tr>
</thead>
<tbody>
<tr>
<td>APP-AuNPs</td>
<td>4.23 µM</td>
<td>0–100 µM</td>
<td>(5)</td>
</tr>
<tr>
<td>TPTS</td>
<td>7 ng/L</td>
<td>0.1–500 ng/mL</td>
<td>(6)</td>
</tr>
<tr>
<td>spectrophotometric</td>
<td>$10^{-10}$ mol/L</td>
<td>0.0047–0.09 µM</td>
<td>(7)</td>
</tr>
<tr>
<td>ICP-MS</td>
<td>1.32 µM</td>
<td>3–133.35 µM</td>
<td>(8)</td>
</tr>
<tr>
<td>AgPA-CHIT</td>
<td>$1.05 \times 10^{-6}$ M</td>
<td>100–300 µM</td>
<td>This work</td>
</tr>
</tbody>
</table>

Determination of Hg$^{2+}$ and Pd$^{2+}$ Ions in Water Samples

To evaluate the practical application of AgPA-CHIT, drinking water and lake water samples from the Hongzi Lake in Qingdao Agricultural University were collected. The water samples were first filtered through a 0.2 µm membrane to remove any suspensions and then spiked with different concentrations of the Hg$^{2+}$ and Pd$^{2+}$ standard solution within the linear ranges. Finally, the spiked Hg$^{2+}$ and Pd$^{2+}$ ions were recovered by the proposed methods. The analytical results are displayed in Table I. The recoveries for the selective detection of Hg$^{2+}$ were in the range of 96.8–100.9%, and Pd$^{2+}$ was in the range of 91.3–101.3%. The relative standard deviations (RSD) of the four measurements were all lower than 2.2%. These results suggested that the proposed method has great potential for the sensing of Hg$^{2+}$ and Pd$^{2+}$ in environmental samples.

Conclusions

In conclusion, a simple, cost-effective, and highly selective onsite colorimetric detection method for Pd$^{2+}$ and Hg$^{2+}$ ions was developed by using green synthesized AgNPs, which was modified by adding organic acid and chitosan. The organic acid with a different reducing power and dissociation degree can tune the synthesis procedure of AgNPs and lead to nanoparticles with different SPR intensities and size distributions. The biological macromolecule chitosan served as a stabilizer and complexing agent, which endowed the system with excellent film-forming properties. Thus, in addition to the color change of AgNPs from pale yellow to colorless and light brown when adding the Hg$^{2+}$ and Pd$^{2+}$ ions, the obtained...
solid film with obvious color changes can also act as a convenient onsite selective detection method of Hg²⁺ and Pd²⁺ ions. This method showed high selectivity to Hg²⁺ and Pd²⁺ than other metal ions with detection limits of 2.26 × 10⁻⁷ M and 1.05 × 10⁻⁶ M, respectively. The detection of Hg²⁺ and Pd²⁺ in real water samples also revealed good detection recoveries. The colorimetric discrimination of Hg²⁺ and Pd²⁺ ions in solvent and solid film provides a new avenue for simultaneous onsite detection of metal ions by the naked eye.

Conflicts of Interest
There are no conflicts to declare.

Acknowledgments
We gratefully acknowledge the financial support from the National Science Foundation of China (21403122) and High-level Science Foundation of China (21403122). We thank the Central Laboratory of Qingdao Agricultural University and the Central Laboratory of Qingdao Agricultural University.

References

Kaiyu Zhang, Yuxin Sang, Qinxing Sun, and Weina Li are with the College of Chemistry and Pharmaceutical Sciences, Qingdao Agricultural University, in Qingdao, China. Direct correspondence to Weina Li at wnli@qau.edu.cn.
FEATURED ARTICLE


Jerome Workman, Jr.

In this Part 4 survey article describing instrument services and testing, we look into spectroscopy electronics, including printed circuit board (PCB) design and manufacturing, a description of spectroscopy instrument design services, a summary of instrument testing services, and a description of the firmware and software aspects of instrumentation. This is the final installment of our four-part instrument component survey series. As promised, we have published tutorial articles, and posted the The Spectroscopy Instrument Components Terminology Guide. We hope our readers found these articles helpful for our “under the hood” look into spectroscopy instrumentation.

In this final installment of our four-part spectroscopy components survey article, we take a closer look at four main topics, covered in four tables, with each table containing the following columns of information content—the instrument component service name, a text description of the service offered, basic specifications (information), and references and links. The previous three parts of this series were published in the March, June, and September issues of Spectroscopy (1–3), with additional references given in the literature (4–7). Table V refers to spectroscopy electronics, including printed circuit board (PCB) design and manufacturing. Table VI describes spectroscopy design services, specifically instrument design and manufacturing services. Table VII summarizes instrument testing services, most notably, electrical safety testing, electromagnetic compatibility (EMC), and electromagnetic interference (EMI) testing. Finally, Table VIII delves into the firmware and software aspects of instrumentation, which include instrument driver and control firmware, instrument function driver software, data transfer and user interface software, and, finally, data analysis software. All component service functions are listed in alphabetical order for each table.

References
(2) J. Workman, Spectroscopy 37(6), 42–45 (2022).

• Continued on Page 31
**TABLE V: Spectroscopy electronics**

<table>
<thead>
<tr>
<th>Component Service</th>
<th>Text Description</th>
<th>Specifications</th>
<th>References and Links</th>
</tr>
</thead>
<tbody>
<tr>
<td>PCB manufacturing</td>
<td>Printed circuit board (PCB) design and manufacturing involves electronic design and layout (including layout dimensional drawings, schematics, bill of materials [BOM], layout file, component placement file, assembly drawings and instructions, and Gerber file [CAD systems layer drawings set]), creation of parts ordering and testing, pick &amp; place equipment for placing all components on the board, and quality inspection and functionality testing.</td>
<td>IPC-2581B Generic Requirements for Printed Board Assembly Products Manufacturing Description Data and Transfer Methodology</td>
<td>PCB manufacturing document: <a href="https://www.ipc.org/TOC/IPC-2581B.pdf">https://www.ipc.org/TOC/IPC-2581B.pdf</a></td>
</tr>
</tbody>
</table>

**TABLE VI: Spectroscopy instrument design services**

<table>
<thead>
<tr>
<th>Component Service</th>
<th>Text Description</th>
<th>Specifications</th>
<th>References and Links</th>
</tr>
</thead>
<tbody>
<tr>
<td>Instrument design</td>
<td>Instrumentation design work generally includes outward form design and esthetics, electronics and PCB design, mechanical design, optical design, and software design. In addition, standard assembly and testing protocols must be completed and final tested for all component parts and final assembled instrumentation. The design package for the final instrument must include layout dimensional drawings, schematics, bill of materials (BOM) with production volume costing, layout file, component placement file, assembly drawings and instructions, and CAD systems drawings. Generally one or more prototype versions of an instrument system will be produced, tested and refined prior to the manufacture of the final production model. Instruments must undergo PASS labeling, electrical and mechanical safety, and electromagnetic compatibility (EMC) testing or electromagnetic field (EMF) testing before commercial sale.</td>
<td>Specify the following: Applications Cost constraints Operating environment Performance requirements Sampling requirements Calibration requirements Optical design Mechanical design Electrical design Software and firmware design Testing requirements Building requirements Components required Development time Create prototype CAD drawings Create prototype Gerber files for PCBs Specify BOM Order parts Build and test prototypes Finalize design Electrical and safety testing Finalize assembly instructions</td>
<td>A. Scheeline, Appl. Spectrosc. 71(10), 2237-2252 (2017). <a href="https://ibsen.com/resources/spectrometer-resources/spectrometer-design-guide/">https://ibsen.com/resources/spectrometer-resources/spectrometer-design-guide/</a></td>
</tr>
<tr>
<td>Instrument manufacturing</td>
<td>Instrument manufacturing involves the in-house or out-of-house (outsourced) quality manufacturing and testing of production volumes of instrumentation, generally for commercial sale. Instruments are built and tested to written specifications as provided by the design and production engineering teams.</td>
<td>Define material and quality requirements Define testing and quality procedures Define costs Define delivery schedule and unit volume requirements</td>
<td>M. Dabhilkar and L. Bengtsson, Prod. Plan. Control 19(3), 212–228 (2008).</td>
</tr>
</tbody>
</table>

**References and Links**

### TABLE VII: Spectroscopy instrument testing services

<table>
<thead>
<tr>
<th>Component Service</th>
<th>Text Description</th>
<th>Specifications</th>
<th>References and Links</th>
</tr>
</thead>
<tbody>
<tr>
<td>Electromagnetic compatibility (EMC) and electromagnetic interference (EMI) testing</td>
<td>EMC and EMI testing measures the ability of electronic equipment to function satisfactorily in its intended use without introducing, or being seriously affected, by electromagnetic disturbance to its environment. EMC/EMI certifications are mandatory in Europe, USA, China, Korea, Australia, and New Zealand.</td>
<td>To comply with EMC Directive 2014/30/EU.</td>
<td>EMC Directive 2014/30/EU document: <a href="https://eur-lex.europa.eu/legal-content/EN/TXT/PDF/?uri=CELEX:32014L0030&amp;rid=4">https://eur-lex.europa.eu/legal-content/EN/TXT/PDF/?uri=CELEX:32014L0030&amp;rid=4</a>.</td>
</tr>
</tbody>
</table>

### TABLE VIII: Instrument software and services

<table>
<thead>
<tr>
<th>Component Service</th>
<th>Text Description</th>
<th>Specifications</th>
<th>References and Links</th>
</tr>
</thead>
<tbody>
<tr>
<td>Control software</td>
<td>This is software that may reside on a standard computer board that is specifically written to control motors, shutters, mirrors, valves, sampling systems, robotics, and other mechanical devices that operate and control instrument functions.</td>
<td>Operating systems such as GNU/Linux, OS X, Windows.</td>
<td>S.R. Nidumolu and M.R. Subramani, Manag. Inf. Syst. 20(3), 159–196 (2003). Tutorial (.pdf): <a href="https://instruct.uwo.ca/chemistry/532/lecture6d.pdf">https://instruct.uwo.ca/chemistry/532/lecture6d.pdf</a>.</td>
</tr>
</tbody>
</table>

Continued on Page 31
Continued from Page 19

Conclusions

We defined PEPs and looked at the synthesis and spectra of a common PEP, cellulose acetate. We found that cellulose acetate follows the ester Rule of Three as expected, and that it clearly exhibits the high wavenumber C-C-O stretch of ester esters found near 1240 cm\(^{-1}\). We then reviewed the spectra of the three types of carbonates: saturated, mixed, and aromatic. Polycarbonates exhibit three intense peaks from C=O, O-C-O, and O-C-C stretching, similar in size and position to the trio of peaks from esters. We looked at the spectrum of pure Lexan and two spectra where it is found in a mixture. The position of the C=O stretch in carbonates may be used to distinguish the three types of carbonates from each other. The C=O of carbonates is much higher than most esters making carbonates easy to spot. To distinguish between saturated carbonates and saturated esters, use the fact that saturated carbonates have an O-C-O peak from 1280 to 1240 cm\(^{-1}\), whereas saturated esters have their C-C-O peak from 1210 to 1160 cm\(^{-1}\).

References

Company Description

Alluxa offers and manufactures high-performance optical thin films that are used in wide-ranging applications including life sciences, research, semiconductor, and LIDAR. All of Alluxa’s thin-film optical filters and mirrors are hard-coated using a proprietary plasma deposition process on equipment that was designed and built by our team. This allows us to repeatably produce the same high-performance optical thin films in all of our coating chambers.

Alluxa is an ISO 9001:2008 certified, ITAR registered, optical coating manufacturer located in Santa Rosa, California. Founded in 2007 by a team of thin-film deposition veterans, Alluxa’s core team brings together decades of expertise and diverse backgrounds in deposition, automation, metrology, and optics.

Chief Spectroscopic Techniques Supported

- We support all chief spectroscopic techniques

Markets Served

We serve a wide range of markets including: aerospace, astronomy, automotive, biotechnology, chemical technology, communications, environmental monitoring and sensing, forensic science, imaging, inspection and identification, lighting, machine vision, research, medical and biomedical, microscopy, military, photonics manufacturing, remote sensing, LIDAR, and spectroscopy.
**Company Description**

Since 1936, millions of samples worldwide have been analyzed using LECO instruments for elemental analysis, gas chromatography, spectrometry, hardness testing, optical analysis, and more. We work with our customers to find the right solution for the type of sample analysis they are doing, helping them to achieve data that is clear, consistent, and accurate. Headquartered in St. Joseph, Michigan, USA, LECO has over 25 international offices with additional distributors authorized to sell or service LECO products throughout Europe, Asia, Latin America, and Canada.

**Chief Spectroscopic Techniques Supported**

- Glow Discharge Atomic Emission Spectrometry
- Bulk Quantitative Elemental Analysis
- Compositional Depth Profile Analysis (CDP)

**Markets Served**

LECO glow discharge spectrometers are used in a variety of applications, helping users to determine direct elemental composition or compositional depth profiling for coatings and surface treatments. Markets include metal producers, foundries, surface modification and finishing, government and private materials research, electronics manufacturing, automotive, aerospace, and more.

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**Major Products/Services**

**GDS900 DC Bulk Glow Discharge Spectrometer:** Bulk analysis of solid conductive samples. Well suited for both routine elemental analysis in production settings and laboratories requiring a system capable of analyzing a variety of materials without timely modifications in research and development settings.

**GDS950 DC/RF Bulk and CDP Glow Discharge Spectrometer:** Bulk and compositional depth profile analysis of both conductive and non-conductive samples. This system expands the capability of a spectrometer to quantitative depth profile analysis, providing up to nanometer depth resolution at speeds faster and costs much less of other competitive surface analysis techniques.

**Facility**

Our headquarters in St. Joseph, Michigan, USA, is comprised of several facilities, each dedicated to improving customer success, including state-of-the-art research and development centers and rugged manufacturing facilities. LECO has over 25 worldwide subsidiaries and distributors who are authorized to sell our equipment to over 75 countries around the world.
GFS Chemicals

Company Description
GFS Chemicals is a US-based manufacturer of specialty and fine chemicals serving customers worldwide since 1928. As an ISO 9001:2015 manufacturer, GFS Chemicals manufactures ACS- and reagent-grade materials, including high-purity trace metal acids and salts, AA and ICP standards, dyes, indicators, inorganic and organic fine chemicals, turbidity standards, and other common laboratory reagents. Additionally, GFS manufactures its own line of high-quality Karl Fischer reagents that covers both volumetric and coulometric applications and ISO 17025 NIST-traceable water standards.

Chief Spectroscopic Techniques Supported
● AA
● ICP-MS
● ICP-OES
● UV-vis
● Turbidity

Markets Served
GFS Chemicals is committed to providing the best product at the right price. Our technical staff works to understand the challenges scientists face and delivers custom solutions and products to meet their needs. GFS has delivered results in demanding markets—including food, pharmaceutical, environmental, electronics, clinical, energy, flavors & fragrances, agrichemicals, petrochemical, water, cannabis, and many more. From research laboratory to pilot plant, GFS is here for you.

Major Products/Services
GFS Chemicals offer a product portfolio of proprietary chemicals available in small bottle to drum quantities. GFS’s offering of over 8000 items includes a full range of PPT/PPB trace-grade acids, UV-vis standards, AA/ICP standards, Karl Fischer reagents, turbidity standards, pH buffers, conductivity standards, OHR, GC/HPLC solvents, inorganic salts, and other high-quality reference materials for your QA/QC laboratory. In addition, GFS’ capability to produce specialty alkynes and olefins, pharmaceutical building blocks, trace metal salts and solutions, low moisture and anhydrous salts, and specialty rare earth salts and solutions makes GFS a preferred partner for organizations across an array of industries.
● Trace metal acids, ppt and ppb grades
● Trace metal salts
● UV-vis standards
● AA/ICP standards
● pH buffers
● Turbidity standards for water analysis
● APHA standards
● Conductivity standards
● KF reagents

Facility
GFS Chemicals maintains three manufacturing sites in Columbus, OH. Each specializes in either organic, inorganic, or laboratory reagent manufacturing. The ppt acids are bottled, labeled, and packaged in a class 100 clean room.
What’s Your Time Worth?

Redigesting samples or disassembling an ICP-MS fouled by lower grade acid? Fighting with interferences or a noisy baseline?

"Uptime, not downtime."

When we developed our new Blade Microwave Digestion system, there was a massive shortage of trace metal acid. GFS Chemicals was able to deliver the next day, and their acids exceeded our expectations.

-Sam Heckle, CEM Applications Chemist

Next-Gen Technology.
Sophisticated Process Controls.

In the 60’s, no one could manufacture perchloric acid clean enough to digest lunar samples, so GFS Chemicals built an acid distillation plant to serve the U.S. Space Program, establishing our expertise in high purity acid manufacturing. Our second acid plant was finished in 2021, filling a need for a U.S. based manufacturer that reliably supplies trace metal acids to half of the U.S. population in three days or less. Much has changed over the last fifty years and our entire process is now controlled by cutting-edge technology. Advanced process controls and analytics ensure Veritas Acids are ultrapure every time.
ConcentratIR2™
Introducing the newest member of our family. A multiple reflection diamond ATR for microliter liquid sampling, measuring only 18.5 cubic inches. Small enough to fit in the palm of a child’s hand. Small enough to fit in your spectrometer. Flow and heated options available.

Major Products and Services
Harrick Scientific offers the most complete line of spectroscopy sampling products, including:

- Video MVP—a diamond micro ATR accessory with a built-in camera
- DiaMaxATR—an affordable monolithic diamond ATR accessory
- ConcentratIR2—a compact, multi-reflection horizontal ATR microsampler that utilizes a Si or diamond ATR
- Praying Mantis—a diffuse reflectance accessory available with environmental chambers/reaction cells
- Seagull—a variable angle specular reflection and ATR accessory
- VariGATR—a variable angle grazing angle ATR accessory for monolayers on gold and silicon substrates
- FiberMate 2—an interface between spectrometers and fiberoptic applications
- MultiLoop, Omni-Diff, and Omni-Spec—fiberoptic probes for ATR, diffuse reflection, and specular reflection
- Several types of liquid and gas transmission cells
- Custom design development

Facilities
Harrick Scientific Products is located 30 miles north of New York City in Pleasantville, New York. Our products are also available through FT-IR and UV-vis spectrometer manufacturers, as well as distributors in the United States and throughout the world.

Company Description
Harrick Scientific Products, Inc. specializes in designing and manufacturing instruments for optical spectroscopy. Since being established in 1969, Harrick Scientific has advanced the frontiers of optical spectroscopy through its innovations in all spectroscopic techniques. The founder of the company, Dr. N.J. Harrick, pioneered attenuated total reflection (ATR) spectroscopy and became the principal developer of this technique. Harrick Scientific offers a complete selection of sampling accessories, including both standard and custom designs, as well as an extensive line of optical elements.

Chief Spectroscopic Techniques Supported
- Transmission
- Specular reflection
- Diffuse reflection
- ATR
- Fiber optics

Markets Served
Harrick Scientific serves analytical markets worldwide. Harrick’s customers typically are from research or quality control laboratories of industrial, governmental, research, and academic institutions throughout the world. Industries served include chemical, electronic, pharmaceutical, forensics, and biomedical.
ConcentratIR2™ Introducing the newest member of our family. A multiple reflection diamond ATR for microliter liquid sampling, measuring only 18.5 cubic inches. Small enough to fit in the palm of a child’s hand. Small enough to fit in your spectrometer.

Flow and heated options available.

harricksci.com/ConcentratIR2
Markets Served
Our products are found in a wide variety of global industries including academic, pharmaceutical, forensics, biotechnology, chemical, fuel, defense, food, and environmental.

Manufacturing
All JASCO products are developed and manufactured at our facilities located in Tokyo, Japan.

Company Description
JASCO: The Japanese Spectroscopy Company has been developing precision instruments for molecular spectroscopy and chromatography since 1958.

Molecular Spectroscopy
⦁ Circular Dichroism (Electronic and Vibrational)
⦁ High-Throughput CD
⦁ Circularly Polarized Luminescence (CPL)
⦁ Polarimeters
⦁ FT-IR
⦁ FT-IR Microscopy
⦁ FT-IR Portable
⦁ Raman Microscopes
⦁ Probe Raman
⦁ UV-visible/NIR Spectrophotometers
⦁ UV-vis/NIR Microscopy
⦁ Fluorometers
⦁ Dissolution Tester

Chromatography
⦁ HPLC
⦁ UHPLC
⦁ SFC/E
THE NEXT GENERATION OF FTIR SPECTROMETERS

Introducing the **FTIR-6X**

The sleek design of the new 6X FTIR research-grade spectrometer houses a Michelson interferometer optimized to 28°. A new concept in long lifetime VCSEL lasers and trusted corner-cube mirrors ensure consistent accuracy.

**Designed for applications made both inside and outside the sample compartment.**

- Wide measurement range from the NIR to MIR to FIR with minimal component exchange
- Large sample compartment for any sampling accessory
- Ports to bring light into and out of the instrument for user configurable measurements
- Remote detectors for measurement across custom sampling chambers
- Spectra Manager™ for experimental control and leveraging data
- Excellent signal to noise, purge and vacuum.
Company Description
Ocean Insight is the Applied Spectral Knowledge company. Our mission is to lead in creating precise yet practical optical solutions that enable researchers and industry to solve meaningful problems in health, safety, and the environment.

Ocean Insight provides spectral technologies and application expertise to customers facing measurement challenges for applications ranging from biomedical diagnostics to semiconductor processing. Our business comprises three entities: “core” technologies – spectrometers and accessories first developed under the Ocean Optics brand – for the research and science community and OEM industrial customers; Applied Systems, which uses those core products and other sensing technologies to solve specific industrial challenges; and International Light Technologies, which Ocean Insight acquired in 2022 to expand the company’s light measurement and detection system offering.

Chief Spectroscopic Techniques Supported
UV, visible and NIR; absorbance, transmittance and reflectance; Raman, SERS and fluorescence; laser-induced breakdown spectroscopy; multispectral imaging; absolute and relative irradiance; color measurement; software and algorithm development; fiber optical chemical sensing; calibration and testing.

Markets Served
Ocean Insight technologies are utilized across a diverse range of industries and disciplines including consumer electronics, medical diagnostics, industrial manufacturing, metal recycling, pharmaceutical manufacturing, and semiconductor processing. Our spectral products are used by researchers, developers, industrial engineers and OEM suppliers for lab work, field research, instrument development and process monitoring worldwide. From start-ups to Fortune 500 technology leaders, Ocean Insight partners with businesses to configure, develop and scale spectral solutions that deliver decisive results.

Major Products/Services
Spectrometers: UV, visible and NIR spectrometers; spectrophotometers; fluorescence spectrometers; laser-induced breakdown spectrometers; Raman instruments; industrial spectrometers; reflectometers; field spectrometers; spectral sensors; light meters, radiometers, photometers and spectroradiometers.
Software: Custom software, algorithm development and machine learning.
Solutions: Spectrometers, sensors, fibers and accessories; multispectral cameras; components and subassemblies for embedding into OEM applications; turnkey systems; custom software; in-line, nonferrous scrap metal sorting system; color inspection system; in-line anodization dye monitoring system.
Optical Sensors: Oxygen sensors
Sampling Accessories: Collimating lenses, cuvettes and holders, calibration standards, filters and holders, flow cells, cosine correctors, and integrating spheres.
Light Sources: Deuterium, tungsten halogen, LEDs, calibration sources, excitation sources, lasers, light meters and xenon.
Optical Fiber and Probes: Fiber optic patch cords; custom assembly options; reflection and transmission probes; and vacuum feedthroughs.

Facilities
Ocean Insight has sales, service, engineering, and manufacturing operations in Florida, and has sales locations throughout Europe, Latin America, India, and China. Ocean Insight is a subsidiary of Halma plc, an international market leader in safety, health, and sensor technology.
Remarkable Spectral Performance in a Compact Footprint

The ultra-compact new Ocean ST microspectrometer combines advances in detector technology with smart optoelectrical design to provide spectral performance comparable to a large-bench spectrometer. Use Ocean ST for everyday lab applications, integration into other devices, and setups where space is limited.

Ocean Insight

oceaninsight.com
Company Description
PIKE Technologies was established in 1989, specializing in the development and manufacture of accessories and optical systems that enhance the performance of commercial spectrometers. PIKE concentrates on making the life of laboratory personnel easier.

Chief Spectroscopic Techniques Supported
- Attenuated total reflectance (ATR)
- Diffuse reflection
- Specular reflection
- Transmission, including sample cells and IR windows
- Remote sensing
- High-throughput automation
- Integrating spheres
- Polarization control
- Microscope objectives
- Microsampling
- Gas cells

Markets Served
PIKE products are designed for molecular spectrometers in the petrochemical, food, forensic, biochemical, pharmaceutical, semiconductor, optical, agricultural, and material science industries. In addition, PIKE Technologies specializes in custom design of products for specific applications. PIKE products are built with craftsmanship and care to exceed customer expectations. Visit our website and take advantage of our unique and interactive Crystal Properties Chart and FT-IR Calculator.

Major Products/Services
- IRIS – High performance diamond ATR
- MIRacle™ – Patented universal sampling accessory (Diamond, ZnSe, Ge, and Si)
- HATR – Multiple reflection horizontal ATR
- GladiATR™, GladiATR Vision™ – Heating up to 300 °C and viewing options
- VeeMAX™ – Patented variable angle specular reflection and ATR accessory
- AutoATR – Automated ATR sampling
- Gas Cells – Long and short path
- PressPRO – Automated programmable hydraulic press, 15 and 25 ton
- A wide range of fully automated FT-IR and NIR products with easy-to-integrate AutoPRO™ software

Facility
PIKE Technologies, Inc. is located in Madison, Wisconsin. We distribute directly to our customers worldwide and to OEMs for packaging with spectrometers of all manufacturers. Please call or visit our website for additional product information.
NEW!

MIRacle Peltier
By PIKE Technologies

A new temperature control option for your ATR accessory.

Retrofit your existing MIRacle or configure a new ATR

Take advantage of the perks that the MIRacle Peltier element offers:

- Sub-ambient measurements to 10 °C without a refrigerated liquid circulator, up to 90 °C.
- Fast heating and cooling rates, 10 °C/min and 5 °C/min, respectively.
- Temperature stability, even at room temperature.

To learn more about PIKE Technologies’ latest MIRacle Peltier, visit our website, piketech.com or contact us at info@piketech.com.
Company Description
Moxtek is a leading supplier of advanced nano-optical and X-ray components used in display electronics, imaging, and analytical instrumentation. Moxtek provides innovative, solution-based products and services focused on performance, quality, and value. Moxtek products enable many new scientific discoveries and improve the quality of everyday life.

Moxtek optical polarizers and polarizing beamsplitters enable advancements in projection display and analytical instrumentation including: 2-D and 3-D projection display, near-eye display, and optical analysis instrumentation.

Moxtek X-ray products empower compact handheld and benchtop elemental analysis for positive material identification. Moxtek products are used in various EDXRF, WDXRF, and XRD systems for environmental screening, hazardous substance analysis, and sorting and recycling.

Major Products/Services

X-ray Components
- X-ray Detectors
- X-ray Tubes and Sources
- X-ray Windows

Wire-Grid Polarizers
- Inorganic Wire-Grid Polarizers
- UV-vis-IR Polarizers
- Polarizing Beam Splitters (PBS)
- Pixelated Polarizer Arrays

Applications and Markets Served

X-Ray Components
- Energy Dispersive X-ray Florescence (EDXRF)
- Wavelength Dispersive X-ray Florescence (WDXRF)
- Energy Dispersive Spectroscopy (EDS)
- X-ray Diffraction (XRD)
- Non-Destructive Testing (NDT)
- Microanalysis
- X-ray Radiographic inspection

Facility
Moxtek is headquartered in Orem, Utah. Moxtek designs, develops, and manufactures our products in world-class cleanrooms and facilities. Moxtek has additional processing facilities in Asia with several distributors worldwide.
Company Description
Throughout our 27 year history, REFLEX Analytical Corporation has received considerable attention as the low-cost, high-value provider of spectroscopy supplies and accessories. Although such accolades are gratifying, we are most proud, not of our operational efficiency or the comprehensive nature of our product line, but of the sterling reputation created by our customers. This prevails opportunity to celebrate and thank you, our customers, for your loyalty. Our mission statement remains intact as we look forward to “Serving you across the Spectrum” in the years ahead.

Chief Spectroscopic Techniques Supported
- AA, UV-vis, NIR, and FT-IR spectroscopy
- Fluorescence spectroscopy
- Transmission spectroscopy
- High temperature and high pressure spectroscopy
- HPLC, GC, and ICP mass spectroscopy
- Cryogenic spectroscopy
- Extreme conditions spectroscopy
- ATR reflectance and diffuse reflectance spectroscopy
- Specular reflectance spectroscopy
- Optical and polarization spectroscopy
- Fiber optic spectroscopy
- Remote sensing spectroscopy
- Ultra high vacuum spectroscopy
- XRF spectroscopy

Markets Served
REFLEX Analytical Corporation serves an international analytical community within research and development laboratories at corporations, government agencies, and universities. This same community is involved with investigating and developing new products and enhancing old products in the state of a liquid, solid, or gas. With pride, we provide the means for analytical groups worldwide to successfully launch new products and instill quality within products as they go through their life cycle.

Major Products and Services
- Standard optics and custom optics
- ATR hemispheres-prisms-rods
- Beamsplitters-filters-lenses
- Optical coatings and metallization
- UV-vis-NIR-IR polarizers
- Free-standing wire grid polarizers
- Ultra-high vacuum viewports
- Standard cuvettes and custom cuvettes
- UV-vis-NIR-IR cells
- Fluorimetry, calorimetry, polarimetry, and cytometry cells
- DNA and protein analysis cells
- Blood analysis cells
- Dynamic light scattering cells
- Tungsten halogen lamps
- HPLC and deuterium lamps
- Mercury, xenon, and PID lamps
- Hollow cathode lamps
- Atomic absorption graphite tubes
- Liquid, solid, and gas transmission cells
- High-pressure and high-temperature cells
- Variable temperature cells
- Cryogenic cells
- Online process flow cells
- Fixed pathlength gas cells
- Variable pathlength gas cells
- FT-IR reflectance accessories
- GC capillary columns
- ICP glassware-cones-coils-electron multipliers
- Evacuable and XRF pellet dies
- Solid sampling equipment
- Laboratory presses
- Grinding mills

Facility
REFLEX Analytical Corporation has the establishment of distribution channels through a selected dealer network and seeks to expand representation for their products by inviting contact from dealers and distributors in your area.
Company Description
When OEM system manufacturers around the world require precision and well-regulated high voltage power, one name most often comes to mind—Spellman high voltage.

Over the past 70 years, Spellman has provided innovative system developers with custom-designed high-voltage DC power supplies to meet their unique application requirements.

Spellman boasts the world’s largest and most experienced high-voltage engineering staff, with world-class project teams experienced in specific applications and technologies, dedicated not only to new designs, but also to sustaining engineering throughout the life of each product.

Markets Served
Spellman provides the broadest range of precision high-voltage products for the mass spectrometry, analytical instrumentation, and biotechnology fields. We offer precision high-voltage power supplies with well-regulated outputs from 62 V to 500 kV, and from 200 mW to 200 kW.

Major Products/Services
Mass spectrometry: We offer an extensive portfolio of standard and customized precision high-voltage solutions for the ionization, mass separation, and detection processes. Discrete modules through to complex integrated multiple output supplies are available for “all” high voltages throughout the time-of-flight (TOF), MALDI-TOF, quadrupoles, ICP, ion trap, LC- and GC-MS, and ion mobility instrument types.

Analytical X-ray: We are a world-leading provider of X-ray generators, with a vast portfolio of high-performance, robust and reliable standard and custom product offerings for analytical X-ray applications, including X-ray diffraction and fluorescence. The range includes low-power modules for handheld and portable XRF systems, through to higher power solutions for bench top and standard lone XRF/XRD multi-purpose research instruments.

SEM, FIB, and Analytical Laboratory:
Spellman offers solutions for thermionic and field emission SEM, as well as Ga ion and plasma sources, focused ion beam, and lenses supplies. Additionally, we cover many general analytical applications, including ion pumps, DNA sequencers, CZE, chromatography, and molecular analysis.

Key features of our product range:
- high stability
- fast switching
- multiple outputs
- ppm level performance
- fast polarity reversal
- minimized micro-discharges
- ultra-low ripple
- arc and short circuit protection
- compact footprints with both analogue and digital interfaces
- graphical user interfaces (GUI) to support early developmental work and UL, CE and RoHS compliance.

Facility
Headquartered in the U.S., with facilities in New York, Spellman maintains design, manufacturing, and support in key regions around the world, (New York, Mexico, Germany, UK, China, Korea, and Japan), to provide OEM customers with local technical expertise and rapid response repair capability. All owned facilities are LEED certified; all leased facilities have ISO certification. Ask us about specifics or go to our website: www.spellmanhv.com.
Areas of application include polymer sciences, pharmaceutical research and development, life science, geoscience, thin films and coating analysis, semiconductors, nanotechnology, materials science, and automated particle analysis.

Major Products and Services
The WITec alpha300 R Raman microscope leads the industry in speed, sensitivity, and resolution. These attributes are available simultaneously and without compromise. Speed is provided by the precise mechanical components and cutting-edge electronics, sensitivity is delivered through the optimized optics and detectors, and the exceptional resolution derives from WITec’s inherently confocal architecture and the know-how accumulated in more than two decades at the very forefront of Raman imaging. Confocal Raman imaging microscopes are among the most powerful and versatile instruments available to today’s scientists, and no other product line places the full potential of the technique into the hands of users the way WITec’s alpha300 can. It can be configured as required by a specialized experiment or upgraded as techniques evolve. It features rock-solid stability, the freedom of modularity, and an unequaled level of performance. WITec instruments can also combine different techniques for a more comprehensive understanding of a sample.

Company Description
Since its founding in 1997, WITec has established itself as a market leader in the fields of Raman imaging microscopy and correlative microscopy techniques, including Raman-AFM, Raman-SNOM, and Raman-SEM (RISE). WITec’s innovative spirit has kept the alpha300 microscope series at the forefront of the Raman imaging market since it initially revolutionized the field and established Fast Raman Imaging™ as a standard method. In September 2021, WITec became a member of the Oxford Instruments Group, bringing technology leadership in Raman microscopy to its extensive portfolio of businesses.

Ongoing development of the first truly confocal Raman imaging system continues to enable the setting of benchmarks in sensitivity, speed, and spectral and spatial resolution. As reflected in WITec’s maxim “Focus Innovations” our success is based on continually introducing new technologies and a commitment to maintaining customer satisfaction through high-quality, flexible, and innovative products.

Chief Spectroscopic Techniques Supported
⦁ Confocal three-dimensional Raman imaging microscopy and Raman micro-spectroscopy
⦁ Ultra-fast and Fast Raman Imaging™
⦁ Correlative Raman imaging: AFM, SNOM, fluorescence, or PL
⦁ Topographic Raman imaging (TrueSurface™ microscopy)
⦁ RISE™ microscopy (Raman Imaging & Scanning Electron Microscopy)

Markets Served
WITec microscopy systems are delivered worldwide to academic and industrial research laboratories focusing on high-resolution chemical imaging and materials characterization.
Per- and polyfluoroalkyl substances (PFAS) are a large class of synthetic chemicals that present numerous analytical challenges, including their widespread presence in a variety of environmental samples. In the US, PFAS may contaminate public drinking-water systems that serve an estimated 19 million people. The U. S. Environmental Protection Agency (EPA) is continuing to aggressively implement their PFAS Action Plan—the most comprehensive cross-agency plan ever to address an emerging chemical of concern. The EPA has established a non-enforceable health advisory level of 70 parts per trillion (ppt) for the sum of pentadecafluorooctanoic acid (PFOA) and heptadecafluorooctanesulfonic acid (PFOS) for drinking water. The EPA is developing a potential rapid screening tool to identify total PFAS presence and absence in 2021. This eventual standard operating procedure will be used to quantify total organic fluorine (TOF).

Therefore, a sensitive, fast, and simple TOF detection method is needed for environment pollution monitoring and control. The method is based on a combination of solid-phase extraction (SPE) with high-resolution–continuum source graphite furnace molecular absorption spectrometry (HR-CS GF MAS). In another Application Note, “Determination of Extractable Organically Bound Fluorine (EOF) in Surface Water,” the solid phase extraction (SPE) procedure has been fully discussed for the extraction of fluorinated compounds. HR-CS GF MAS was used to detect total fluorine via in-situ formation of gallium(I) fluoride (GaF) molecules. To achieve the best signal, the furnace tube was conditioned with the molecule forming agent (Ga) and modifiers (Pd/Mg/Zr/Ba) before the sample was injected. From the literature, it’s known that melting point/vapor pressure of the fluorinated compounds significantly impacts the recovery rates of the different compounds. Thus, the drying and pyrolysis procedure in the furnace program were optimized to keep possible losses of fluorinated compounds as low as possible. To evaluate the optimization approach, 24 different fluorine compounds were mixed for the QC sample. These 24 compounds were selected with different numbers of fluorine atoms and boiling points. Calibration strategies were developed to obtain the best recovery rate for this QC sample.

Conclusion
In this study, a fast, easy, and sensitive complementary method for total fluorine analysis in wastewater is presented. This study shows that the MAS method can be successfully applied using the contrAA 800 G for the measurements. The optimized furnace program and calibration strategy provide high sample throughput, sensitivity, and accuracy. Only 3.5 min/replicate is needed for each sample. A 100% recovery rate of QC sample is successfully achieved with an inorganic and organic mixture calibration strategy. The lowest LOD of 4 ppb is also achieved using the inorganic and organic mixture calibration strategy. The results of fluorine determination by HR-CS-GF MAS show good reproducibility and long-term stability. Sample dilution and spiking can be easily achieved with an AS-GF autosampler. No additional cleaning steps are required for this method.

Method Development Strategy
For the quantification of fluorinated organic compounds as a sum parameter, a species-unspecific response of high-resolution continuum source graphite furnace molecular absorption spectrometry (HR-CS GF MAS) was developed.
In this application note, a novel signal averaging technique is utilized that dramatically improves signal to noise ratio (SNR) performance in a high resolution spectrometer. With higher SNR comes better quality spectra and more accurate results.

In spectrometers, SNR is a function of several factors, some more easily managed than others. For example, in a PC-based spectrometer setup, signal averaging to improve SNR can be carried out in operating software on the host computer, but that can take longer to process than what may be acceptable for your application.

High Speed Averaging Mode (HSAM) is a hardware-accelerated signal averaging function now available for use with newer-model Ocean Insight spectrometers that overcomes those limitations by enabling many more spectral averages over a given time period, yielding a much higher SNR per unit time. This can be important for time-critical and real-time applications, where decisions must be made very quickly and with a high degree of certainty.

Experimental Setup
We tested the advantage that HSAM offers by measuring the relative output of an 880 nm LED using an Ocean HR2 UV-visible high resolution spectrometer with 600 µm optical fibers and attenuator. This was a useful area within the spectral range to evaluate, as in some silicon CCD-array detector setups, the spectral response at NIR wavelengths may drop off as grating dispersion efficiency and detector quantum efficiency drop off.

HSAM is a function accessible via Ocean Insight’s OceanDirect device driver platform. OceanDirect provides a library of additional functions that allows user to write custom software for use with Ocean Insight spectrometers.

Results
In one sense, what HSAM accomplishes is to “pull” signal out of the noise. This is demonstrated in Figure 1, where we compared the 880 nm LED measurement results for a single average scan, which is quite noisy; then for 1000 scans (less noise); and finally, for 10,000 scans (minimal noise).

Summary
The big advantage to accessing HSAM in OceanDirect is that users can perform more spectral averages, over less time, than with OceanView spectrometer operating software alone. For example, OceanView can process 10,000 averages in about 2 s. But because HSAM performs the averages directly on the hardware, OceanDirect can process 10,000 averages in about 200 ms —10x faster. This can enhance SNR for existing applications markedly and open up new application possibilities.
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**New Peltier Cooled Cyclonic Spray Chamber**

Glass Expansion is pleased to release a new and improved Peltier Cooled Cyclonic (PCC) Spray Chamber Kit designed to be fully compatible with the Agilent® 7900 and 8900, in addition to the legacy Agilent® ICP-MS models. According to the company, the PCC provides improved washout and increased sample throughput compared to the standard Scott-style spray chamber.

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REFLEX Analytical’s new development in sealed liquid transmission cell sampling is Restriction of Hazardous Substances (RoHS) compliant. According to the company, this development eliminates the lead and mercury amalgam seal normally associated with older sealed liquid transmission cell designs. The new RoHS advanced design uses leak-free fluoropolymer seals that are isolated from the liquid sample. Available in static and flow through configurations with pathlengths ranging from 0.015–10mm, each cell offers a 13 mm aperture. The liquid flow through transmission cells are assembled with 1/8” compression fittings. Choose from a variety of transmission window materials.

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