Vol. 31 No. 1 February/March 2019

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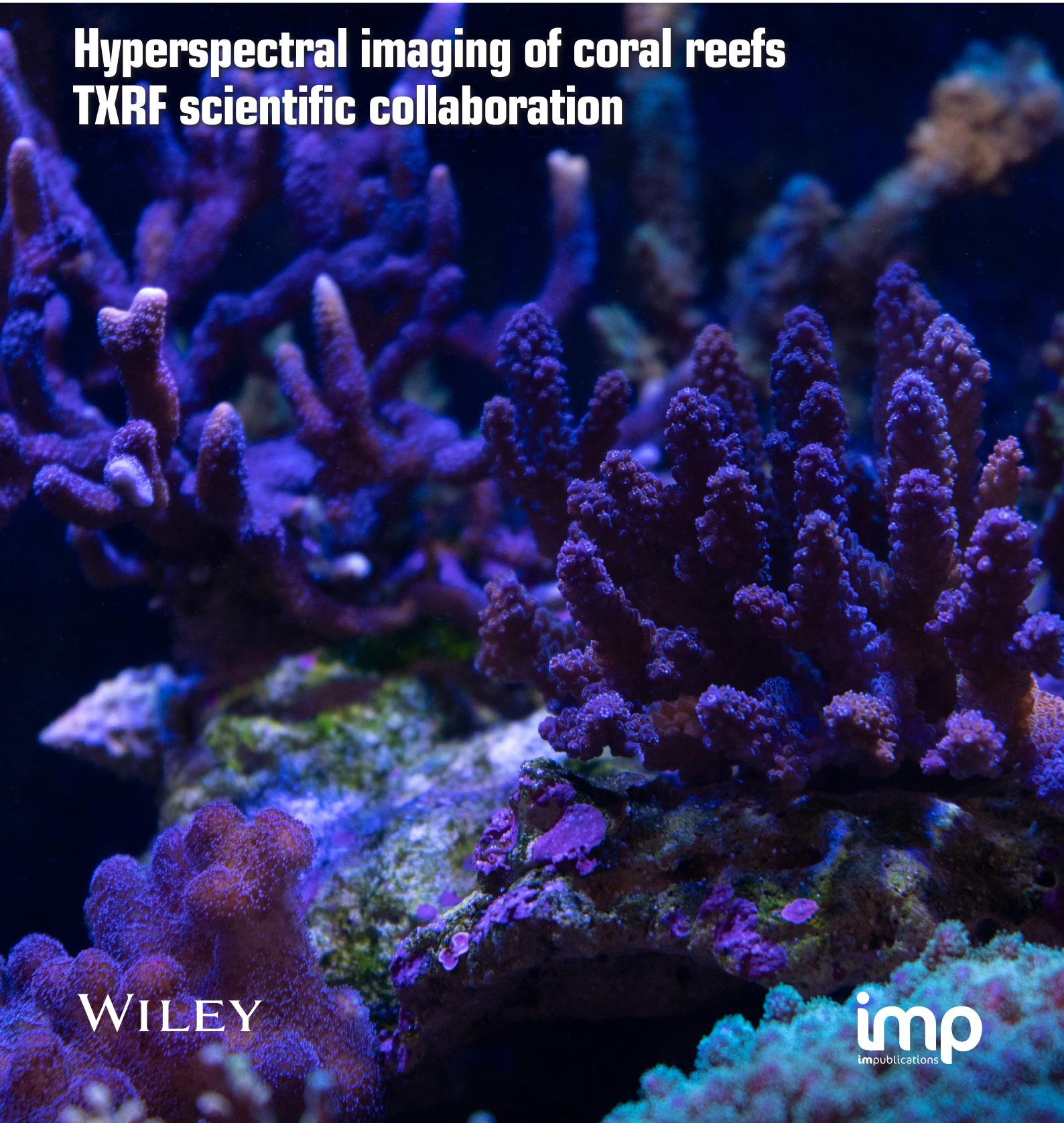
Hyperspectral imaging of coral reefs
TXRF scientific collaboration



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EDITORIAL

Climate change

It seems that practically every day we hear of further examples of the disastrous effects of climate change. Coral reefs have been used as examples for decades, since the "bleaching" caused by corals stressed by heat expelling their symbiotic photosynthesising algae is such a dramatic effect. In our first article, Jonathan Teague, Jack Willans, Michael Allen, Thomas Scott and John Day describe their work in developing a hyperspectral imaging system that can be deployed on a submersible remotely operated vehicle to monitor coral health through changes in their natural fluorescence.

Ramón Fernández-Ruiz tells us about the "TXRF Workgroup: an alternative environment for scientific collaboration". Total reflection X-ray fluorescence (TXRF) is a "Cinderella" technique: not widely known but with great potential. Ramón and other members of the TXRF Workgroup are making strenuous efforts both to spread the word about TXRF and to improve communication within the TXRF community. As Ramón points out, atomic absorption or plasma spectroscopies may be the "go to" techniques for many, but TXRF is worthy of consideration.

In the Tony Davies Column, Hafiz Azeem and Tony take us back to climate change. The world is moving away from reliance on fossil fuels and towards the use of biomass, but there is a hidden danger of fires developing from bulk stores of material such as straw waste. Interestingly, smoke from burning or smouldering plant-based material has a specific signature from a marker of cellulose combustion. Hafiz has developed a technique based on thermal desorption with gas chromatography-mass spectrometry to detect very low levels of the marker, well before the smoke would set off a normal smoke detector. This can also be used to detect the burning of rainforests, another climate change issue!

Kim Esbensen concludes his first series of Sampling Columns that have concentrated on the theory and understanding of the importance of representative sampling. Don't worry, Kim will be back with more columns but looking at practical examples. So, if you have a particular representative sampling problem, let me or Kim know!

Coral reefs are suffering from the effects of climate change. A hyperspectral imaging system fitted to a submersible remotely operated vehicle has been developed and can be used to assess coral health based on induced fluorescence. Find out in the article starting on page 12.

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Spectroscopy Europe is a joint publication of John Wiley & Sons Ltd, The Atrium, Southern Gate, Chichester, West Sussex PO19 8SQ, UK, and IM Publications LLP, 6 Charlton Mill, Charlton, Chichester, West Sussex PO18 0HY, UK.

Vol. 31 No. 1
February/March

ISSN 0966-0941

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Spectroscopy Europe is a controlled circulation journal, published seven times a year and available free-of-charge to qualifying individuals in Europe. Others can subscribe at the rate of €152 (Europe), £108 (UK), $208 (ROW, postage included) for the seven issues published in 2016. All paid subscription enquiries should be addressed to: *Spectroscopy Europe*, John Wiley & Sons Ltd, Journals Administration Department, The Atrium, Southern Gate, Chichester, West Sussex PO19 8SQ, UK.

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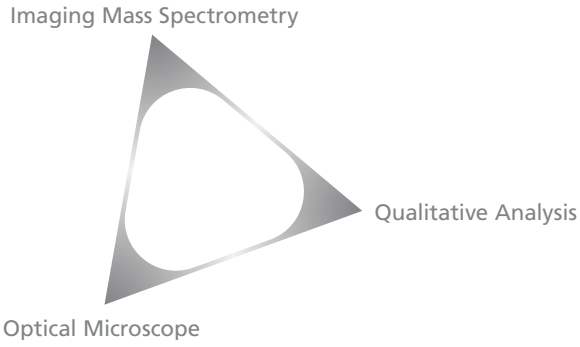

Broad application fields
such as medical research, pharmaceutical development and food analysis

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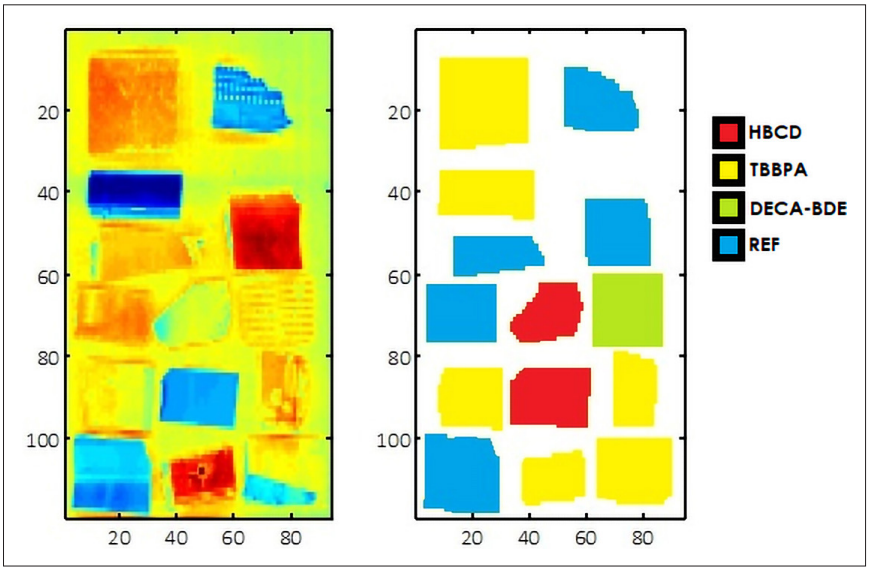
Improved plastics recycling with NIR hyperspectral imaging

If we are ever to reduce the quantity of plastics being dumped into the environment, efficient recycling is essential. Currently, many plastics cannot be economically sorted to enable their recycling. For example, many plastics contain flame retardants to increase their resistance to ignition, reduce flames spreading, minimise smoke formation and to prevent the plastic from dripping. The amount of flame retardant added to plastics and the type used can vary considerably, due to the need to tailor the plastic to its particular application and to meet safety standards. However, only plastics of the same type and with similar flame retardants can be recycled together. Therefore, before recycling can occur, plastics need to be sorted, not only by the type of plastic (acrylonitrile butadiene styrene and polystyrene in this study) but also by any flame retardant added. Without sorting, recycling cannot take place.

In a paper published in *JSI—Journal of Spectral Imaging* (doi: https://doi.org/10.1255/jsi.2019.a1), José Amigo and co-authors detail a method using near infrared hyperspectral imaging and chemometrics that can sort between different types of plastic and between different additions of flame retardant. Using an imaging technique for this recycling application is important, since it can identify individual pieces of plastic and any flame retardant they may contain from among many others, for example, on a conveyor belt in a recycling plant.

For optimum performance, any sorting technique needs to be fast and able to identify accurately the wide range of combinations of plastic and flame retardants it may encounter. The system reported in the *JSI—Journal of Spectral Imaging* paper uses the Decision Trees chemometrics technique combined with spectral data obtained from near infrared hyperspectral imaging and is able to distinguish between different plastics and flame retardants within them with 100% accuracy.

José Amigo commented "Recycling plastics has been studied for many years. Indeed, some commercial cameras separating a limited number of plastic types have been available for some time. However, in this research, we wanted to go a step further to separate plastics containing flame retardants. Moreover, the proposed methodology was tested with real samples that can be found in current recycling lines."

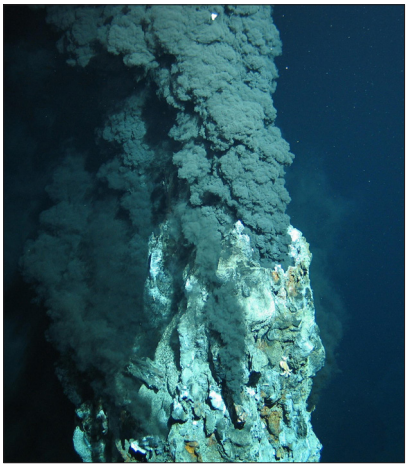


Near infrared hyperspectral imaging of samples of plastics and their classification as a function of type of flame-retardant: 1,2,5,6,9,10-hexabromo-cyclododecane, HBCD (red samples); 3,5-tetrabromobisphenol A, TBBPA (yellow samples); Pentabromophenyl ether, Deca-BDE (green samples); and reference, REF (blue samples).

LIBS measurement on the deep-sea floor

For the first time, scientists at the Laser Zentrum Hannover e.V. (LZH) have succeeded in measuring zinc samples at a pressure of 600 bar using laser-induced breakdown spectroscopy (LIBS). They were able to show that the LIBS system developed at the LZH is suitable for use in the deep sea at water depths of up to 6000 m.

Locating mineral resources on the sea floor has so far been rather expensive. In order to reduce the costs, the LZH is working with eight other European partners to develop a laser-based, autonomous measuring system for underwater use by 2020. The system is intended to detect samples, such as manganese nodules, and analyse their material composition directly on the deep-sea floor.



The measurement of elements with LIBS should help to locate natural resources in a non-destructive way in the future. Photo: GEOMAR (CC BY 4.0).

For this purpose, the scientists at the LZH are developing a system for LIBS within the scope of the EU ROBUST project. In order to test the LIBS system developed by LZH under deep-sea conditions, a special pressure chamber was designed and manufactured. This can simulate a water depth of 6500 m with a pressure of up to 650 bar. The chamber is suitable for both freshwater and saltwater. Through a viewing window, the laser radiation enters the

pressure chamber with the test sample to be analysed.

New EPR method for analysing metalloproteins

A new electron paramagnetic resonance (EPR) method only needs a very small liquid sample to analyse metalloproteins. This was developed by a research team led by Associate Professor Eiji Ohmichi and Tsubasa Okamoto at the Kobe University Graduate School of Science. The findings were published in *Applied Physics Letters* (doi: https://doi.org/10.1063/1.5055743).

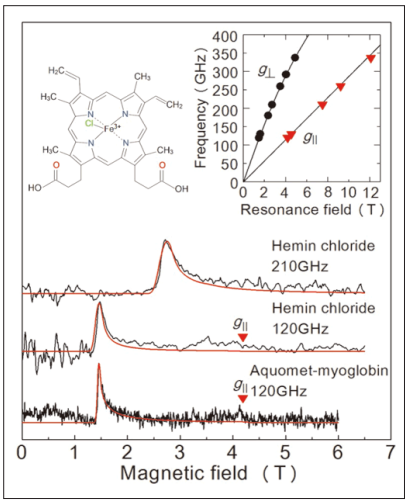
Metalloproteins play vital roles in our bodies for oxygen transport and storage, electron transport, oxidation and reduction. In many cases, the metal ions in these proteins are the active centres for these activities, so by identifying the exact state of these ions, we can understand the mechanisms behind their functions. EPR can be used to measure the state of electron ions in proteins. Effective EPR techniques require a certain amount of specimen volume for sensitive measurements. However, many metalloproteins are difficult to isolate and refine, so we can only obtain small samples.

Conventional EPR measurements detect the electromagnetic waves absorbed by metal ions. The notable feature of this study is the use of a trampoline-shaped device called a nanomembrane. In EPR the electron spin transitions to a high-energy state by absorbing electromagnetic waves, but at the same time the spin direction reverses, and the magnetic properties of the metal ions also change. Before the experiment the research team attached tiny magnets to the nanomembrane, so the changes in the force of attraction between the magnets and the metal ions are transformed into a force on the nanomembrane, and this EPR signal is detected. Since the nanomembrane is very thin (just 100 nm) we can sensitively measure small changes in force that accompany EPR absorption.

The solution specimen is placed in a solution cell directly above the membrane. The cell volume is 50 µL, and the team adds about 1–10 µL of solution for measurement. In order to prevent the solution from evaporating, the cell is covered with a resin lid. In this method the thin and fragile nanomembrane is independent from the solution cell, making it easy to switch specimens.

In order to evaluate the performance of this setup, the team carried out EPR measurement over a high-frequency (over 0.1 THz) for the iron-containing protein myoglobin and its model complex haemin chloride (see Figure). The team succeeded in detecting EPR signals across a wide wave frequency (0.1–0.35 THz) for a 50 mM concentration, 2 µL haemin chloride solution. They also observed a characteristic EPR signal for an 8.8 mM, 10 µL specimen of myoglobin solution. A great advantage of this method is the ability to measure across a wide frequency range, making it applicable for metalloproteins with a variety of magnetic properties.

Professor Ohmichi commented: "This new method makes it possible to determine to a detailed level the state of the metal ions in a tiny amount of metalloprotein solution. We may be able to apply the method to metalloproteins that previously could not be measured. For example, in our metabolisms, a metalloprotein called peroxidase plays a crucial role by converting hydrogen peroxide into water, making it harmless, but the details of the mechanism for this reactive process are still unclear. The results from this study can potentially be applied as a leading analysis method to shed light on this sort of vital phenomenon."



Results of the EPR measurements obtained in this study from a frozen solution sample. The top two diagrams are for haemin chloride, and the graph at the bottom is for myoglobin. The red line is a projected signal from a value simulator. The solution concentrations and sample volumes were 50 mM, 2 µL for hemin chloride and 8.8 mM, 10 µL for myoglobin. Measurements took place at 4.2K. By examining the two lines in the upper right graph they are able to determine the exact state of iron ions. The upper left graph shows the molecular structure of hemin chloride.

Mass spec of blister fluid diagnoses burn severity

Diagnosing burn depth, which can continue to increase even hours after the injury initially occurs, takes up to two weeks and often depends on the doctor's experience. Deep burns and those requiring longer than 21 days for healing typically require skin grafts. If doctors could accurately estimate burn depth and time for re-epithelialisation at an earlier stage, they might be able to reduce scarring. This is especially important for paediatric burn patients, because excessive scar tissue cannot expand with the growing child and could hamper joint movements and bone development.

As reported in the *Journal of Proteome Research* (doi: https://doi.org/10.1021/acs.jproteome.8b00355), mass spectrometry was used to analyse the proteomes of 56 samples of blister fluid from burns of different depths and re-epithelialisation times. The researchers found that the deepest burns had a different pattern of protein abundance than shallower ones. For example, haemoglobin protein levels increased with burn depth, which could result from enhanced blood cell damage. Fluid from burns that took longer than 21 days to re-epithelialise had more collagen proteins, which are involved in scar formation, than faster-healing burns. The team found that taking into account the abundance of several proteins was more accurate in predicting burn depth and time to re-epithelialisation than any protein alone. The analysis also revealed several burns that appear to have been misclassified by doctors, suggesting that

the new approach could more accurately diagnose burns at an earlier stage.

Pulsed DNP greatly increases NMR sensitivity

MIT researchers have developed a way to dramatically enhance the sensitivity of nuclear magnetic resonance spectroscopy (NMR). Using this new method, scientists should be able to analyse in mere minutes structures that would previously have taken years to decipher, says Robert Griffin, the Arthur Amos Noyes Professor of Chemistry. The new approach, which relies on short pulses of microwave power, could allow researchers to determine structures for many complex proteins that have been difficult to study until now.

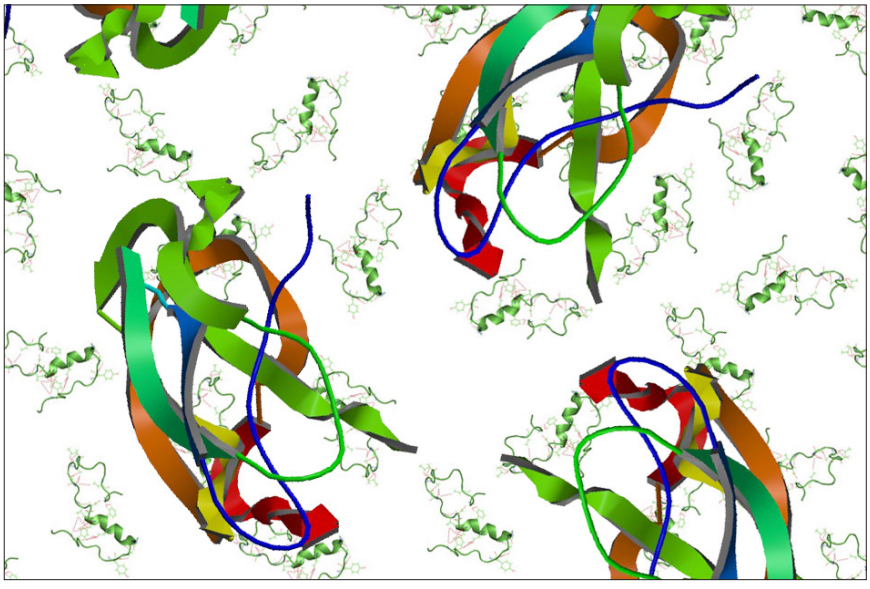
"This technique should open extensive new areas of chemical, biological, materials and medical science which are presently inaccessible", says Griffin, the senior author of the study. MIT postdoc Kong Ooi Tan is the lead author of the paper, which was published in *Science Advances* (doi: https://doi.org/10.1126/sciadv.aav6909). Former MIT postdocs Chen Yang and Guinevere Mathies, and Ralph Weber of Bruker BioSpin Corporation are also authors of the paper.

The sensitivity of NMR depends on the atoms' polarisation. The greater the polarisation, the greater sensitivity that can be achieved. Typically, researchers try to increase the polarisation of their samples by applying a stronger magnetic field, up to 35Tesla. Another approach, which Griffin and Richard Temkin of MIT's Plasma Science and Fusion Center have been developing over the past 25 years, further enhances the polarisation using dynamic nuclear polarisation (DNP). This technique involves transferring polarisation from the unpaired electrons of free radicals to hydrogen, carbon, nitrogen or phosphorus nuclei in the sample being studied.

DNP is usually performed by continuously irradiating the sample with high-frequency microwaves, using a gyrotron. This improves NMR sensitivity by about 100-fold. However, this method requires a great deal of power and does not work well at higher magnetic fields that could offer even greater resolution improvements. To overcome that problem, the MIT team came up with a way to deliver short pulses of microwave radiation, instead of continuous microwave exposure. By delivering these pulses at a specific frequency, they were able to enhance polarisation by a factor of up to 200. This is similar to the improvement achieved with traditional DNP, but it requires only 7% of the power, and unlike traditional DNP, it can be implemented at higher magnetic fields.

"We can transfer the polarisation in a very efficient way, through efficient use of microwave irradiation", Tan says. "With continuous-wave irradiation, you just blast microwave power, and you have no control over phases or pulse length."

With this improvement in sensitivity, samples that would previously have taken nearly 110 years to analyse could be studied in a single day, the researchers say. One major area of interest is the amyloid beta protein that accumulates in the brains of Alzheimer's patients. The researchers also plan to study a variety of membrane-bound proteins, such as ion channels and rhodopsins. Because the sensitivity is so great, this method can yield useful data from a much smaller sample size, which could make it easier to study proteins that are difficult to obtain in large quantities.



MIT chemists have enhanced the resolution of nuclear magnetic resonance (NMR), which should allow more rapid and detailed study of proteins such as the beta amyloid protein that accumulates in the brains of Alzheimer's patients. Image: MIT News

Raman-on-chip for high-throughput, high-resolution handheld spectroscopy

imec will present an on-chip solution for Raman spectroscopy at SPIE BIOS and SPIE Photonics West 2019 in San Francisco. This is based on a newly patented concept providing high optical throughput and high spectral resolution. The solution could pave the way for affordable high-end handheld Raman spectroscopy devices. Imec is looking for technology partners and IDMs to further develop the technology into a commercial application.

It is difficult to develop handheld solutions with the necessary performance for high-end applications, largely because of the limited scaling capacity of conventional dispersive Raman spectrometry whereby scattered light is focused on a slit. Scaling while maintaining high spectral resolution (<1nm) means reducing the size of the slit which immediately limits the optical throughput. imec's new concept, for which a patent is pending, uses massive parallelisation of waveguide interferometers integrated monolithically on top of a CMOS image sensor.

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Developed by the Scripps Center for Metabolomics, METLIN Mass Spectral Database by Wiley is the most complete MS/MS database in the field. With content divided into 3 libraries – experimental spectra, in-silico spectra, and searchable chemical structures – METLIN by Wiley has optimized its searching capabilities and validated spectrum quality to ensure the broadest coverage available.

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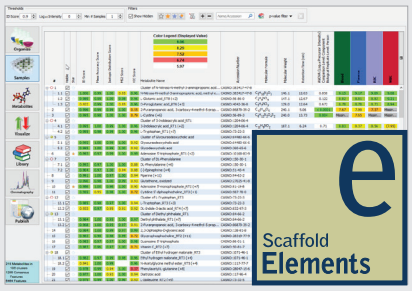

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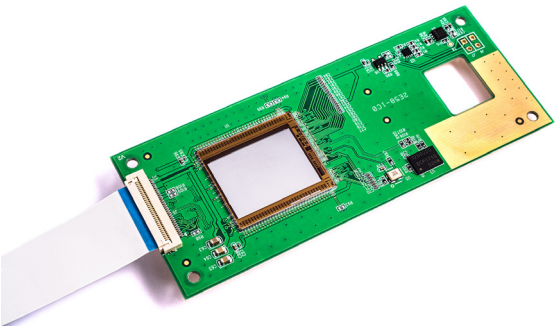


This enables both high optical throughput and high spectral resolution in a miniaturised device. Part of the work was performed under the EU-funded IoSense programme.

Pol Van Dorpe, principal member of the technical staff at imec: "We are very pleased to have achieved this milestone which can mean a breakthrough for the general applicability of Raman spectroscopy. One could even think about smartphone integration. With the right partners we see many application opportunities in areas like food analysis, melanoma detection or skin hydration. In the medical domain, we see opportunities for in-line measurements during surgery or endoscopy. And for space exploration, the ability to perform material analysis with a compact system is of tremendous value."

NIR pocket-size food scanner

Researchers at the Fraunhofer Institute for Optronics, System Technologies and Image Exploitation IOSB, the Fraunhofer Institute for Process Engineering and Packaging IVV, the Deggendorf Institute of Technology and the Weihenstephan-Triesdorf University of Applied Sciences are developing a compact food scanner based on near infrared (NIR) spectroscopy to determine the ripeness and shelf life of produce.

"Foodstuffs are often counterfeited—for example, salmon trout is sold as salmon. Once suitably trained, our device can determine the authenticity of a product. It can also identify whether products such as olive oil have been adulterated", says Dr Robin Gruna, project manager and scientist at Fraunhofer IOSB. However, the system can only evaluate the product quality of homogeneous foods. To enable the analysis of heterogeneous products such as pizza, the scientists are investigating high-spatial-resolution technologies such as hyperspectral imaging and fusion-based approaches using colour images and spectral sensors.

A compact food scanner based on NIR spectroscopy will help avoid unnecessary food waste. © Fraunhofer IOSB

To be able to determine the quality of food based on the sensor data and the measured NIR spectra, and compute shelf-life predictions, the research teams are developing chemometric methods. "Through machine learning, we can increase the recognition potential. In our tests, we studied tomatoes and ground beef", says Gruna. For example, we used statistical techniques to correlate the measured NIR spectra of ground beef with the rate of microbial spoilage and derived the remaining shelf life of the meat from the results. Extensive storage tests, whereby the research teams measured microbiological quality and other chemical parameters under various storage conditions, showed good correlation between the computed and actual total germ counts.

The scanner sends the measured data via Bluetooth to a database in the cloud for analysis. Then the test results are transmitted to an app that displays them to the user and shows how long the food item will remain fresh under different storage conditions, or indicates that its shelf life has already expired. In addition, the consumer is given tips on alternative ways of using food that is past its best-before date. A test phase is due to begin in supermarkets early in 2019, which will investigate how consumers respond to the device. More broadly, it is expected that the versatile technology will be used throughout the value chain, from raw material to end products.

The scanner has the potential to be used for many other applications where NIR spectroscopy can be applied. For example, it could be used to sort, separate and classify plastics, wood, textiles and minerals. "The range of potential applications is very wide; the device just needs to be trained accordingly," says Gruna.

2D-IR spectroscopy probes ions interacting with biomolecules

DNA and RNA are charged polymers with their negative charges located in the molecular backbone, which consists of ionic phosphate (PO_2^-) and of sugar groups (Figure 1). Stabilisation of the macromolecular structures of DNA and RNA requires a compensation of strong repulsive electric forces between the equally charged phosphate groups by ions of opposite, i.e., positive charge. In this context, magnesium (Mg^{2+}) ions are particularly relevant as they not only stabilise the structure, but also mediate the recognition of external binding partners and act as catalytic centres. Moreover, changes of macromolecular

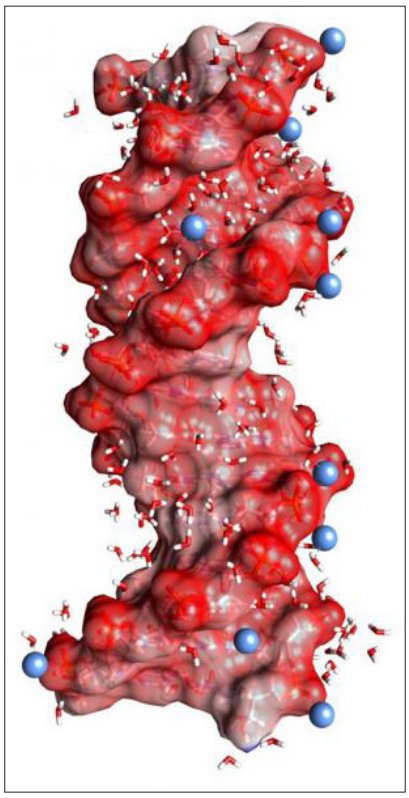


Figure 1. DNA double helix embedded in water (angled small molecules, not to scale). The dark red spheres on the helix surface represent oxygen atoms of the negatively charged PO_2^- units, the blue spheres positively charged ions in the environment. Credit: MBI Berlin

structure via dynamic folding processes are connected with a rearrangement of positive ions embedded in the surrounding water shell.

Positive ions are arranged in different geometries around DNA and RNA: in so-called site-bound or contact-pair geometries, a positive ion is located in direct contact with an oxygen atom of a phosphate group. In contrast, the so-called outer ion atmosphere consists of positive ions separated by at least one layer of water molecules from the phosphate groups. The functional role of the different geometries and the underlying interactions are far from being understood. A deeper insight at the molecular level requires highly sensitive probes which allow for discerning the different ion geometries without disturbing them, and for mapping their dynamics on the ultrafast time scale of molecular motions.

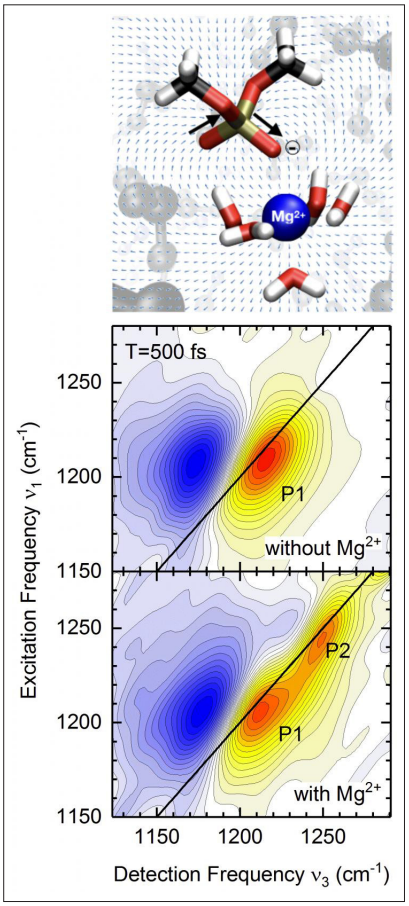


Figure 2. Top: molecular structure of a contact ion pair consisting of dimethylphosphate (DMP) and a magnesium ion Mg^{2+} embedded in water. The arrows mark the elongations of the phosphorus-oxygen bonds in the asymmetric PO_2^- stretching vibration. Bottom: two-dimensional infrared (2D-IR) spectra of the asymmetric PO_2^- stretching vibration measured at a waiting time $T = 500$ fs after vibrational excitation. The vibrational response is shown as a function of the infrared excitation and the detection frequencies and consists of a component P1 from DMP molecules without a magnesium ion in the neighbourhood and the contribution P2 from contact ion pairs. The latter is shifted to higher frequencies due to the interaction between PO_2^- and Mg^{2+}. Credit: MBI Berlin

In a recent publication in *J. Phys. Chem. Letters* (doi: https://doi.org/10.1021/acs.jpclett.8b03568), researchers from the Max Born Institute (MBI) demonstrate that vibrations of phosphate groups represent sensitive and non-invasive probes of ion geometries in a water environment. Dimethylphosphate [DMP, $(CH_3O)_2PO_2^-$], an established model system for the DNA and RNA backbone, was prepared in liquid water with an excess of Mg^{2+} ions (Figure 2, top) and studied by non-linear vibrational spectroscopy in the femtosecond time domain. The experiments make use of two-dimensional infrared (2D-IR) spectroscopy.

The experiments map Mg^{2+} ions in direct contact with a PO_2^- group via a distinct feature in the 2D-IR spectrum (Figure 2, bottom). The interaction with the Mg^{2+} ion shifts the asymmetric PO_2^- stretching vibration to a frequency which is higher than in absence of Mg^{2+} ions. The lineshape and the time evolution of this new feature reveal fluctuations of the contact ion pair geometry and the embedding water shell on a time scale of hundreds of femtoseconds while the contact pair itself exists for much longer times (~ 10^{-6} s). An in-depth theoretical analysis shows that the subtle balance of attractive electrostatic (Coulomb) forces and repulsive forces due to the quantum-mechanical exchange interaction govern the frequency position of the phosphate vibration.

The ability of 2D-IR spectroscopy to characterise the short-ranged phosphate-ion interaction in solution provides a novel analytical tool that complements currently available structural techniques. An extension of this new approach to DNA and RNA and their ionic environment is most promising and expected to provide new insight in the forces stabilising equilibrium structures and driving folding processes.

Quantum sensors improve sensitivity of magnetic resonance

The QUTIS group at the UPV/EHU has participated in a piece of international research together with the CSIC and the University of Ulm in Germany and has produced a series of protocols for quantum sensors that could allow images to be obtained by means of the nuclear magnetic resonance of single biomolecules using a minimal amount of radiation. The results of the research have been published in *Physical Review Letters* (doi: https://doi.org/10.1103/PhysRevLett.122.010407).

With the help of quantum sensors, nuclear magnetic resonance (NMR) has been adapted to work in the nanoscale regime, where it has both the potential to impact many disciplines, such as life sciences, biology, medicine and to provide measurements of incomparable precision and sensitivity. In particular, "we expect that the combination of quantum sensors and dynamical decoupling techniques allows NMR imaging of single biomolecules", said the authors, among whom are Dr Jorge Casanova (Ikerbasque researcher) and Ikerbasque Professor Enrique Solano, at the Quantum Technologies for Information Science (QUTIS) group of the UPV/EHU's Department of Physical Chemistry, as well as researchers of the CSIC, and the University of Ulm (Germany). This quantum-enhanced NMR "will be able to resolve chemical shifts in tiny picolitre samples, producing biosensors with unparalleled sensitivity and providing new insights into the structure, dynamics and function of biomolecules and biological processes", they added.

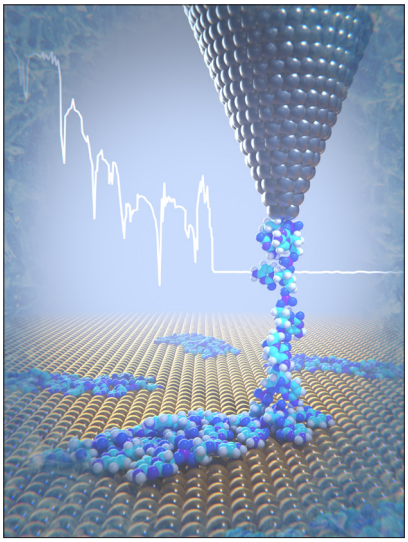
In this context, a fundamental tool to improve the sensitivity of NMR setups is to apply large magnetic fields "that polarise our samples, enhance the signal and increase coherence", they pointed out. This strategy is used, for instance, in MRI, where the human body is subject to large magnetic fields generated by superconducting coils. There are, however, problems when interfacing these samples with our quantum sensors, "because our samples may oscillate much faster than our sensor can follow".

In this work, the authors developed a protocol to allow a quantum sensor to measure the nuclear and electronic spins in arbitrary samples, even when they happen in large magnetic fields. These methods use a low-power microwave radiation to bridge the energy difference between their sensor and the sample.

"The protocol is robust and requires less energy than previous techniques. This not only extends the operation regime of the sensor to stronger magnetic fields, but also prevents the heating of biological samples that would result when using conventional protocols and microwave powers. As a consequence, this work opens a new research line and paves the way for the safe use of nanoscale NMR in the study of biological samples and large biomolecules," said the authors.

Cryo-force spectroscopy reveals the mechanical properties of DNA components

DNA is not only a popular research topic because it contains the blueprint for life, it can also be used to produce tiny components for technical applications. In a process known as DNA origami, scientists can manipulate the genetic material in such a way that folding the DNA strands creates tiny two- and three-dimensional structures. These can be used, for example, as containers for pharmaceutical substances, as conductive tubes and as highly sensitive sensors. To be able to form the desired shapes, it is important to be familiar with the structure, the elasticity and the binding forces of the DNA components being used. These physical parameters cannot be measured at room temperature, because the molecules are constantly in motion. The same is not true at low temperatures: the team led by Professor Ernst Meyer from the Swiss Nanoscience Institute and the University of Basel's Department of Physics have now used cryo-force microscopy for the first time to characterise DNA molecules and examine their binding forces and elasticity.



At low temperatures, a DNA strand is removed from the gold surface using the tip of an atomic force microscope. In the process, physical parameters such as elasticity and binding properties can be determined. (Image: University of Basel, Department of Physics)

The scientists placed DNA strands, only a few nanometres long, containing 20 cytosine nucleotides on a gold surface. At a temperature of 5 K, one end of the DNA strand was then pulled upwards using the tip of an atomic force microscope. In the process, the individual components of the strand freed themselves from the surface little by little. This enabled the physicists to record their elasticity as well as the forces required to detach the DNA molecules from the gold surface.

"The longer the detached piece of DNA, the softer and more elastic the DNA segment becomes", explains lead author Dr Rémy Pawlak. This is because the individual components of the DNA behave like a chain of multiple coil springs connected to one another. Thanks to the measurements, the researchers were able to determine the spring constant for the individual DNA components. Computer simulations clarify that the DNA is detached discontinuously from the surface. This is due to the breaking up of bonds between the cytosine bases and the DNA backbone from the gold surface, and their abrupt movements over the gold surface. The theoretical elasticity values correlate very closely with the experiments and confirm the model of serially arranged springs.

The studies confirm that cryo-force spectroscopy is very well suited to examining the forces, elasticity and binding properties of DNA strands on surfaces at low temperatures.

"As with cryogenic electron microscopy, we take a snapshot with cryo-force spectroscopy, which gives us an insight into the properties of DNA," explains Meyer. "In future, we could also make use of scanning probe microscope images to determine nucleotide sequences."

The researchers reported their findings in *Nature Communications* (doi: https://doi.org/10.1038/s41467-019-08531-4).

ARTICLE

Applied marine hyperspectral imaging; coral bleaching from a spectral viewpoint

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With climate change and other stressors impacting our seas and oceans, coral reef degradation has been brought to the forefront of the climate change issue. Coral reefs are critically important for the ecosystem goods and services they provide. The health of these systems represents a significant concern for the 275 million people who live in coastal tropical and subtropical nations (within 30 km of corals where livelihoods and food security is largely dependent on corals.[1,2] Coral reefs can be incredibly valuable, for example Cruz-Trinidad *et al.*[3] calculated one small reef (10 × 20 km) in the Philippines had an estimated value of $38 million USD/year. This example fiscal valuation only scratches the surface of any reef's true value as an irreplaceable source of food and natural sea defence to developing countries.[4]

Corals are very susceptible to disease and conditions synonymous with climate change, as they have low tolerance to stresses such as varying water temperature, salinity and increased solar irradiation. Coral disease is one of the largest causes of reef degradation and coral death. Its incidence has been increasing worldwide since first observed in the 1970s, particularly in the Caribbean, Red Sea and Indian Ocean, linked in part to declining water quality, declining fish stocks, heat stress and, more recently, to ocean acidification driven by anthropogenic activity.[5–7] With reports of coral disease incidences increasing from 20% to 80% in a three-year period,[7] closer monitoring and protection of this valuable natural asset is essential.

The causes of coral bleaching are widely accepted as a general response to external factors or triggers (stressors) such as elevated water temperature, usually accompanied by increased solar irradiation, ocean acidification or bacterial infection.[8] With these stressors becoming ever more present, mass bleaching events are becoming more frequent, with the first described in 1984 by Glynn and since then a further three global bleaching events have been described in 1998, 2010 and 2015/2016.[9] The most recent mass bleaching event (2015–16) affected 75% of the globally distributed locations surveyed by Hughes *et al.*[10] and is therefore comparable in scale to the then-unprecedented 1997–1998 event, when 74% of the same 100 locations experienced bleaching. With global climate-driven bleaching events coinciding with the El Niño–Southern Oscillation (ENSO) phases, average tropical sea surface temperatures are warmer today under La Niña conditions than they were during El Niño events only three decades ago.[11] This means that predicted climate change and ocean warming scenarios will herald an increase in the frequency of extreme heating events on coral reefs.

Corals primarily responsible for building modern reefs are hermatypic corals, belonging to the group Scleractinia or Stoney corals. Hermatypic corals contain photosynthetic algae specifically dinoflagellates called zooxanthellae, belonging to the genus *Symbiodinium*, that live symbiotically within its cells. The relationship is mutually beneficial, the algae provides the corals with energy from photosynthesis and in exchange receives protection and nutrients needed to conduct photosynthesis (Figure 1). Ahermatypic corals do not possess this symbiosis but instead use other means to survive.[12]

Hermatypic coral communities exhibit a natural fluorescence both from the coral itself and its symbiotic partner. The significance of this is not yet known, several studies have been conducted to try and derive meaning from this and have suggested many possibilities for the role that fluorescent proteins (FPs) play: including (i) acting as a sunscreen by providing a photobiological system for regulating the light environment;[13] (ii) as a host stress response, through their action as antioxidants; or (iii) to attract prey.[14] All that is known is that downregulation of FPs frequently occurs in injured or compromised coral tissue.[15]

The presence of FPs and their behaviour as a response to stress can potentially be exploited as a method for measuring coral health. Analysis of the natural variability in fluorescence intensity for a given species, as well as the differences between diseased and healthy specimens, enables the development of an index relating fluorescence to disease.[16]

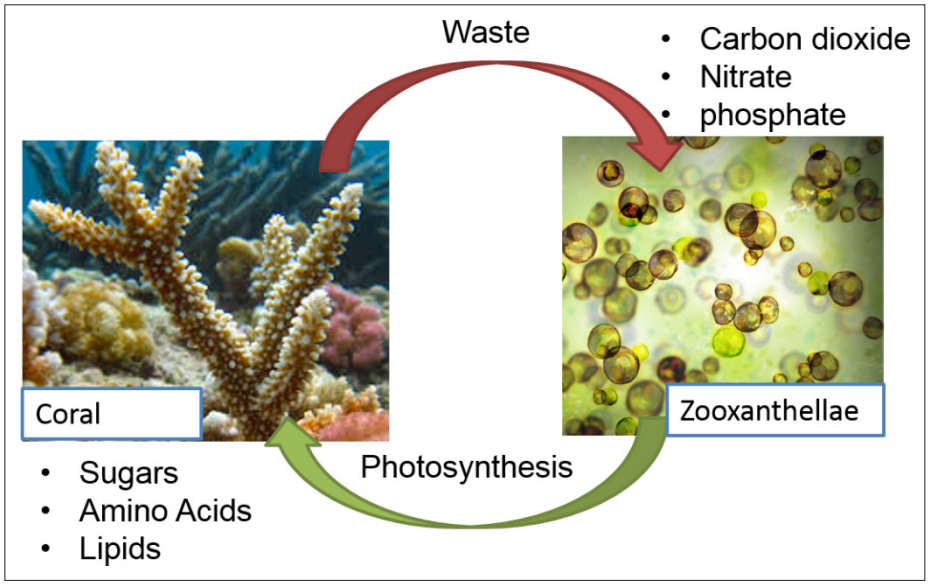

Figure 1. The symbiotic relationship between hermatypic corals and *Symbiodinium*.

Proof of concept and hyperspectral imaging

In order to characterise the subtleties of this natural fluorescence, coral samples at the London Aquarium, provided by coral aquarist Jack Willans, were imaged using a push-broom type hyperspectral camera (Headwall Nano, USA).

This hyperspectral camera captures light across the entire visible (vis) spectrum and some of the near infrared (NIR) (400–1000 nm) in each pixel, but separates the incoming photon (light) flux based on a wavelength, separating the incident light intensity into a large number (hundreds) of spectral bands whilst illuminated by a light source [fluorescence in coral requires ultraviolet (UV) or blue light (400–480 nm)]. This allows the characteristic excitation/emission peaks of coral fluorescence to be determined. Every pixel once processed in the image contains full spectral data relating to that pixel, allowing for the peak wavelength of any observed fluorescence detailed to be determined. The data was processed within the camera to produce a hypercube which could then be viewed in ENVI (Version 5.3.1) (post processing software). Spectra were extracted from various points on each coral sample to determine its emission spectrum.

As Figure 2 shows, the spectra recorded from the corals extracted from the hypercube image indicated that the corals sampled mostly fluoresced in the cyan or green wavelengths (485–512 nm). Samples were selected to represent several different types of corals (branching, plate, soft), including corals known for exhibiting fluorescence and those that were not.

The primary observed fluorescence peaks were used to correlate coral species with emitted colour. Corals exhibiting the colour "cyan" (as classed by Alieva *et al.*)[17] ranged from 459 nm to 516 nm, but with peak fluorescence intensity mainly around 480 nm. Some of the corals did not produce any fluorescence, such as C5, C7, C12, C13, C20 and C22. These made for comparison against actively fluorescing coral spectra. Some of the coral samples exhibited other weaker emission peaks, displaying the presence of dual colour fluorescence, such as C2, which displayed a main peak at 445 nm (cyan) and weaker one at 510 nm (green). Many of the corals exhibited wide emission peaks indicating that multiple colours were emitted by their fluorescence. Many of the spectra show another peak (after 643 nm) which is ascribed to the fluorescence of the coral's symbiotic partner zooxanthellae.

Bleaching experiment

Having gained proof that hyperspectral imaging had the potential to observe and quantify coral fluorescence, we looked at applying this technique for the detection of bleaching. Coral bleaching refers to the process by which the dysbiosis (breakdown of the symbiotic relationship) of zooxanthellae and the host coral occurs. The process of this dysbiosis is usually the expulsion of the zooxanthellae cells from inside the corals cells where they are typically stored. Depending on the stressor, the rate of bleaching varies but is usually a quick process (can be a matter of hours) in individual colonies and can lead to coral cell death or necrosis as a means of extraditing its once partner.

In order to observe and record the bleaching phenomenon, a laboratory experiment was devised where by coral samples (*Montipora digitata*) provided by London Aquarium, were placed into an experimental tank containing artificial sea water at a starting temperature of around 24 °C. The temperature was then incrementally increased by +2 °C each week for four weeks until the temperature reached >30 °C (this is the point at which bleaching occurs by temperature). The coral samples were imaged using the hyperspectral camera

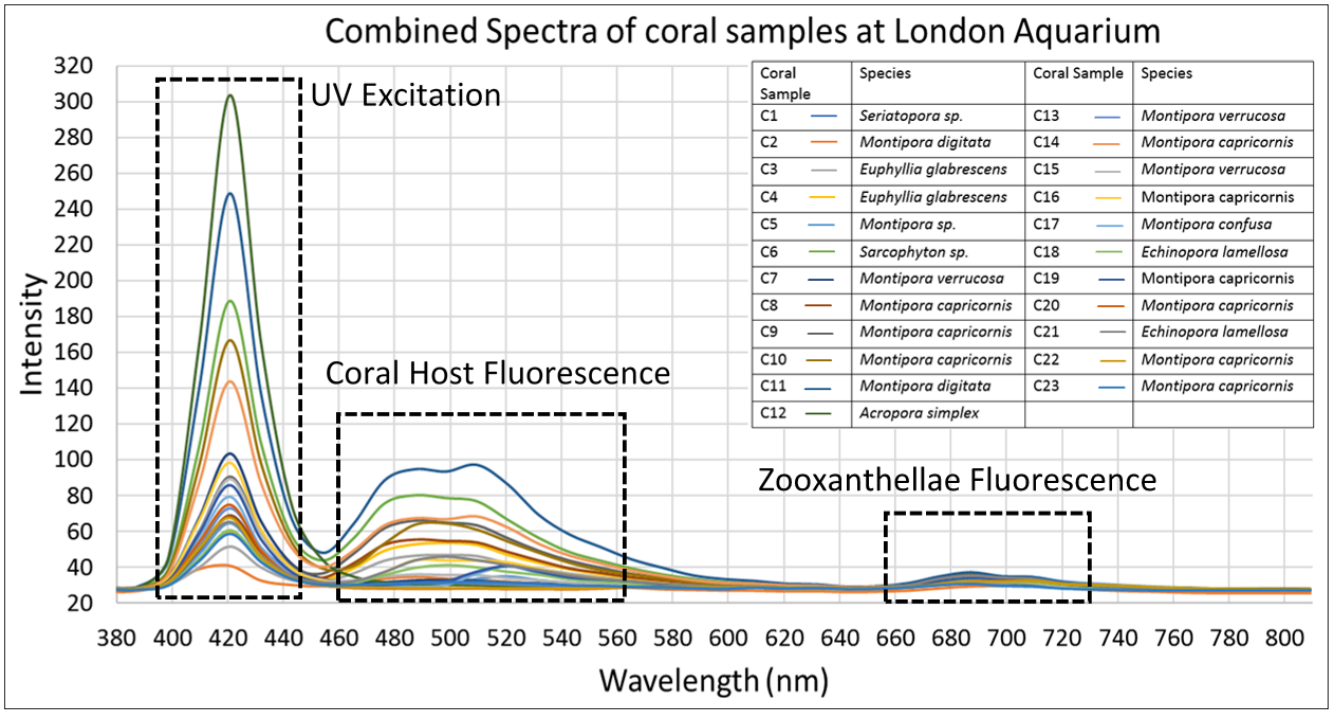

Figure 2. A combined plot of spectra generated from hyperdata generated from areas of interest highlighting all fluorescence visible. Areas of UV excitation and coral and zooxanthellae fluorescence are highlighted.

system at regular intervals throughout the course of the experiment. This purpose was to document the bleaching effect of expulsion of zooxanthellae by monitoring the fluorescence signal which was expected to decrease as they were expelled. The overall health of the coral also degrades due to the bleaching effect and this can also be monitored using the same technique, but looking at the fluorescence peak of the FPs present as opposed to the chlorophyll cells in the zooxanthellae. The collected hyperspectral data from the Headwall nano camera could then be compiled into a hypercube and loaded in to ENVI.

The coral samples for the bleaching experiment were imaged in three light conditions; under white light (Aquarium light bar), blue light (Aquarium light bar 440 nm) and UV light (BlueRobotics UV light pod 405 nm). Under white light illumination, the corals' colour can be seen to decrease in intensity as bleaching progressed, which provides a baseline akin to that of a traditional coral health survey looking at light reflectance. The colour draining of the coral is a process that can be qualitively observed by eye but using hyperspectral methods we can quantify this loss. The blue light illumination elicited the highest intensity of cyan and green fluorescence but masked some of the coral fluorescence signal in the tail of the excitation peak. The UV lights provided a sharper emission peak over the blue light enabling the whole unmasked fluorescence peak to be seen. The experiment allowed us to observe the bleaching process from a quantifiable spectral data perspective as shown in Figure 3.

Conclusion and future work

This study was able to detect fluorescence in corals of numerous different species and identify the spectral intricacies as well as observing coral bleaching from a spectral perspective. The results of this initial research

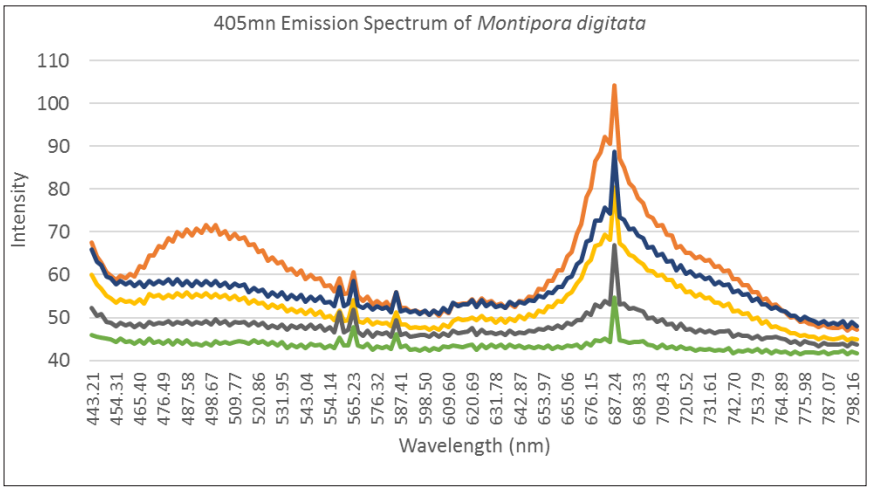

Figure 3. A spectral observation of the "bleaching effect", as the temperature increases observed fluorescence in both the host tissue and zooxanthellae decreases.

provide compelling evidence to prove that fluorescence may be used to indicate coral reef health. The next stage is developing a field deployable system, sufficiently cheap and semi-automated such that reef systems can be automatically and rapidly assessed on a repeated basis.

The field deployable system will be in the form of a portable fully waterproof low-cost hyperspectral imaging system (payload) that can be mounted to an ROV (remotely operated vehicle) (BlueROV2, BlueRobotics) which will act as a stable platform for obtaining images, similar to that provided by drone (UAV) systems in agricultural applications.

The system is required to be "low-cost" (<£10 k) to reduce the high associated costs of commercially available hyperspectral systems and reduce the capital risk of operating in the underwater environment. In order to do this, the monochrome camera (AtikHorizon, Horizon), which ultilises a continuously variable filter, is mounted directly, using a custom 3D printed bracket, on the 16 MPixel CMOS sensor. The filter (LV VIS NIR bandpass filter from Delta Optical Thin Films) has a continuous relationship between the spectral characteristics and the position. The filter has a centre wavelength range between 450 nm and 850 nm. Using a continuously variable filter allows for a standard camera to be modified into a "push broom" hyperspectral camera at very little cost.

The system is then to be deployed over a live reef to gather *in situ* spectral data in order to assess coral health based on the induced fluorescence (Figure 4). Data will be collected in a similar way to existing drone (UAV) technologies with raster pattern flight paths in order to fully cover the whole reef with enough overlap between images to achieve reliable stitching and production of large area maps, and photogrammetry reconstruction of reef topography to produce three-dimensional models of reefs. This will enable the creation of rapid coral health assessments and a spectral library of coral species known fluorescence emission and fluorescence signatures at various stages of bleaching.

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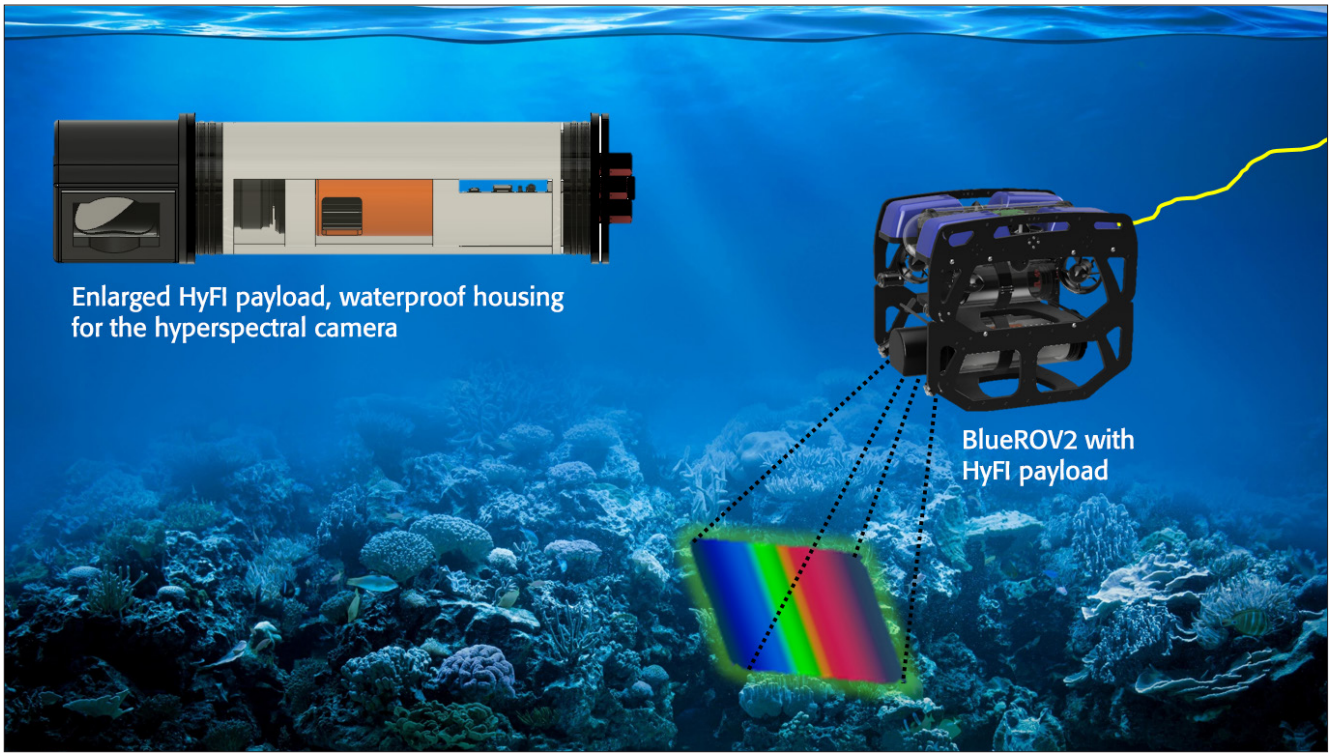

Figure 4. The hyperspectral fluorescence imaging (HyFI) payload, mounted on BlueROV2. Imaging around 1 m above the reef will provide an impact free rapid health assessment. The camera is housed in a custom waterproof housing with a 90° mirrored lens to allow for perpendicular imaging of the reef.

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ARTICLE

TXRF Workgroup: an alternative environment for scientific collaboration

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Introduction

Total-Reflection X-Ray Fluorescence (TXRF) is an X-ray spectrometric technique which has developed from the classic energy dispersive X-ray fluorescence (ED-XRF). Perhaps because both techniques have sometimes been confused and thought of as equivalents, TXRF is little known or widely used when compared with other, more conventional, techniques such as atomic absorption (AAS) or plasma (ICP) spectroscopies. The geometric variation of the Source–Sample–Detector system, which differentiates TXRF from conventional ED-XRF, introduces drastic consequences in physical and analytical aspects. Figure 1 show the main geometrical differences of the ED-XRF and TXRF techniques.

The total reflection condition is obtained when an incident electromagnetic wave is completely reflected by a surface. This occurs for angles lower than a critical angle characteristic of the material of the reflector. Working in the condition of total reflection implies the generation of a field of X-ray standing waves (XSW) over the surface of the sample-carrier reflector, due to the constructive interaction of the incident monochromatic beam and the totally reflected beam. So, a sample deposited over the surface of the reflector, at first approximation, is excited twice, once by the incident X-ray beam and again by the reflected beam. This fact implies an amplification of the atomic X-ray fluorescence signals together with a simultaneous and drastic minimisation of the background (see Figure 2).[1]

As result, TXRF is a "micro-analytical" technique, because only small amounts of sample, around 0.1–10 µg, properly deposited inside the XSW region over the reflector are analysed. The sample is deposited in a thin layer with thickness between 0.1 µm and 10 µm, depending on the kind of material being analysed. Under these conditions, the matrix effects due to absorption and secondary excitation are negligible and the model of infinitely thin film can be applied. So, a simple linear relation between net intensity and concentration can be used. From the analytical point of view, this is by far the biggest advantage that TXRF has over conventional XRF. The TXRF elemental range includes the simultaneous detection of around 72 elements from Al (Z=13) to U (Z=92). Absolute detection limits are of only a few picograms for the great majority of the detected elements or, as relative detection limits, concentrations of few parts per billion (ppb) (µg L^{-1}). As result, the relative sensitivities in TXRF have a universal character, regardless of the analysed matrix. This fact allows the use of the quick and easy method of internal standard addition as the usual way for multi-elemental quantification by TXRF.

The combination of low detection limits, multi-elemental character, micro-analytical capacity, high sensitivity, low times of spectra acquisition and the ease of qualitative, mass proportions and quantitative analysis, open the field

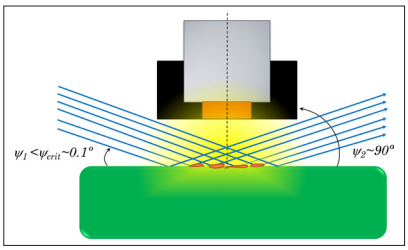

Figure 2. Cross section around the surface of a reflector, showing the field of standing waves (XSW) triangular region and a sample deposited inside it.

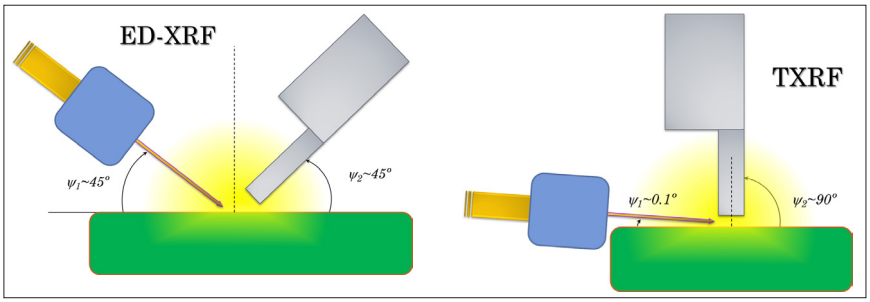

Figure 1. Geometrical arrangement for conventional ED-XRF and TXRF. Ψ_1 is angle of incidence and Ψ_2 angle of detection.

of the analytical application of TXRF to the research of metallic traces in all kinds of complex, and not so complex, systems. Besides that, TXRF has the ability to quantify any liquid or solid samples adequately suspended, without acid leaching, and by simply adding an internal standard and then depositing on an adequate reflector. This implies quick, low cost and no consumption of chemicals for TXRF analysis.[2] In this way, TXRF is a technically consolidated spectroscopy which is more and more applied in very diverse scientific fields and different materials. Many applications of TXRF have been developed—for example, nanoparticle characterisation,[3] catalytic processes studies,[4] biomedicine,[5] physics of materials,[6] archaeometry,[7] forensics,[8] food,[9] environment[10] and many others. TXRF is a powerful tool, still to be discovered within the fields of biomedicine, metallomics and biochemistry as well as in materials, environment, analytical and food sciences.

The TXRF Workgroup

Given the relatively small base of TXRF spectroscopy, the TXRF Workgroup was created to act as a forum for current users and to broaden the usage of the technique. This article explores the aims of the TXRF Workgroup and is based on the invited talk given at the 15th TXRF Conference (TXRF2013) in Osaka, Japan.[11] The TXRF Workgroup uses the power of Social Networks, increasingly present in our lives, for scientific communication, interaction and collaboration.

Present challenges for TXRF spectrometry

Considering my own experience in the field of TXRF,[12] scientists and researchers are frequently influenced by three important factors: bibliography, personal experiences and external suggestions. Such influences can be a hindrance when new techniques, such as TXRF, are presented as an option. This impedes the development of new, alternative and even more appropriate analytical solutions that could be developed by TXRF. As a consequence, TXRF still remains largely unknown in scientific, academic and industrial sectors. So what challenges are holding back the development of TXRF? The *first challenge* facing TXRF is to try to widen an understanding of the analytical pros and cons of TXRF in the industrial and scientific sectors as well as within wider society. The second challenge can be found by analysing the number of scientific publications, with TXRF as a keyword, over time (see Figure 3).

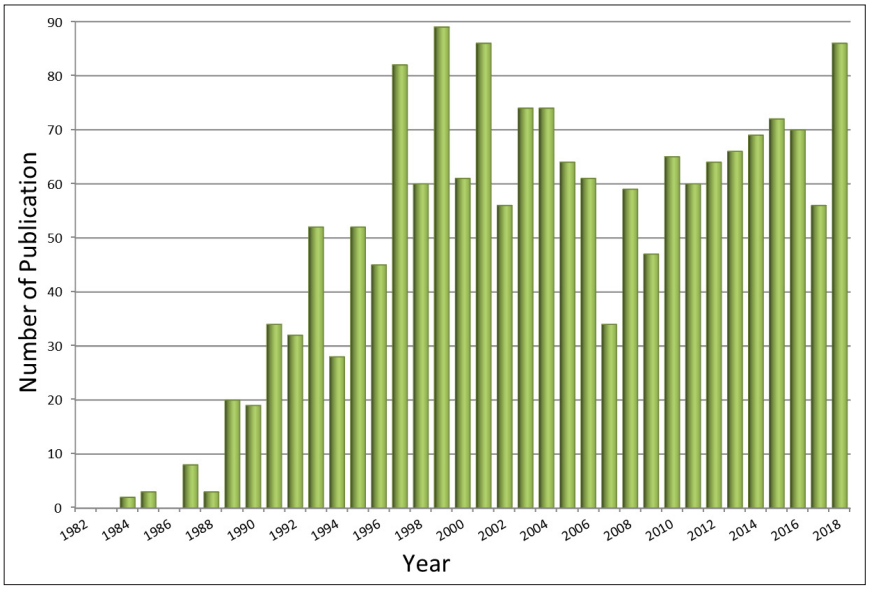

Figure 3. Number of publications per year where the keyword "TXRF" is present in SciFinder.

As might be expected, following the commercialisation of the first TXRF instruments, from the late 1980s to 2000, the trend was upward, within understandable fluctuations, and indicated a promising future for the new spectrometry. However, from 2000 to now, the number of publications has stabilised at around 60 per year. So, the *second challenge* for the TXRF should be try to increase the number of scientific publications. The *third challenge* is related to the wide geographical dispersion of the TXRF community; TXRF needs to find a working environment where distances can be eliminated. The *fourth challenge* can be found in the small number of users of TXRF instruments around the world, especially when compared with other techniques such as ICP-MS, AAS or ICP-OES which have been adopted much more easily in the analytical academic, scientific and industrial world than TXRF. The TXRF community needs to try to increase the number of TXRF instruments in operation. Finally, the *fifth challenge* is related to the small size of its scientific community and, as a consequence, the small number of applications developed in the field of TXRF. Figure 4 shows the number of publications associated with some analytical techniques found for 2018 in the SciFinder database. Around 3962 contributions were published for ICP-MS, 1387 for AAS, 1059 for ICP-OES, 608 for LA-ICP-MS and "only" 89 for TXRF. So, we can see that researchers typically demand the analysis of their samples mainly by ICP-MS, ignoring the fact that TXRF could be an alternative and powerful analytical technique. So, the *fifth challenge* for the TXRF should be to try to increase significantly the number of applications developed and, more importantly, recognised under international accredited quality assurance norms (ISO, ASTM etc.). The first steps have already being taken in this direction by the TXRF community in the last few years.[13] Recently, a European COST action (CA18130) was approved with the name "European Network for Chemical Elemental Analysis by Total Reflection X-Ray Fluorescence" (ENFORCE-TXRF). Its main objective is to introduce TXRF spectrometry in industrial, scientific and wider contexts.

These challenges are significant, so what can we do? From my humble point

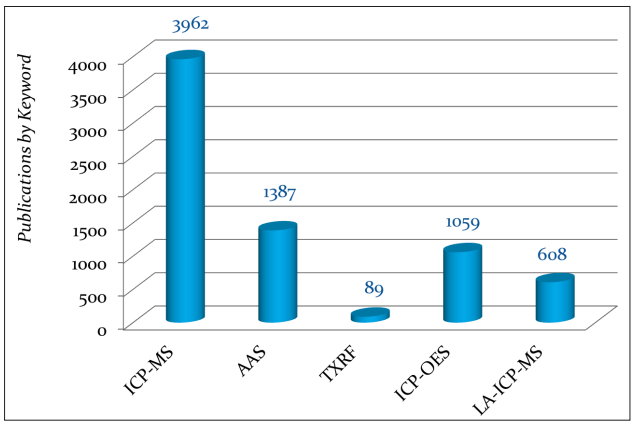

Figure 4. Number of publications related with each one of the technique keywords during year 2018.

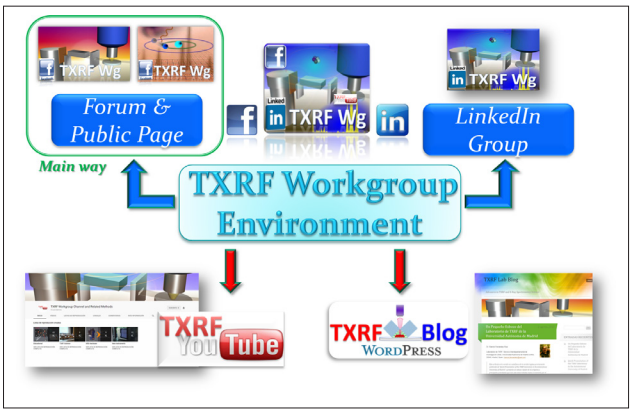

Figure 5. Present structure of the TXRF Workgroup Environment.

of view, a first step to confront them can be found through the interrelation of very diverse disciplines and also by simplifying collaboration between TXRF professionals and with those of related techniques. In this way, even though the number of TXRF professionals are few, each one with limited resources and widely dispersed around the world, we can use the tools that social networks offer to share our resources and knowledge, and generate new knowledge. These ideas were the seeds that motivated me to create the TXRF Workgroup.

TXRF Workgroup description

Nowadays, the TXRF Workgroup is an open discussion and sharing platform where all people are welcomed regardless of their academic level, technological or scientific resources. Only one condition is required to become part of the group as a member, a clear interest in the TXRF-XRS area. One of the basic principles of the group is that the greater the diversity of its members, the higher will be the exchange of ideas between them and, as a natural consequence, the easier should be the generation of new knowledge—the main reason for the TXRF Workgroup. Facebook was the first social network platform we used due, mainly, to their approximately 2300 million users around the world and especially for its ease of use and ability to share digital objects. Today, LinkedIn, YouTube and a WordPress Blog can also be used by any member (see Figure 5). In Facebook, the TXRF Workgroup has two areas of interaction at different levels: a members-only area and a public one. The first, and most important, is the TXRF Workgroup Forum.[14]

This Forum is a restricted Facebook group which only previously approved members can access. Within this Forum it is possible to open lines of discussion, collaboration and/or communication for all members. Also, it is possible to share notes, pictures, articles, links, videos, comments, related news and events of interest, congresses, seminars etc. In parallel, there is a second interaction zone, known as TXRF Workgroup Public Page,[15] which is the public face of the TXRF Workgroup. On this page, anyone can access the information published and where their "followers" are automatically notified of new publications. Recently, a YouTube Channel named the "TXRF Workgroup Channel and Related Methods" has been created.[16] Currently, this contains approximately 43 videos related to all the aspects of x-ray spectroscopy. The idea is that all XRS professionals can suggest and, indeed, include interesting videos in this channel, whether ones they have produced themselves or are already on the Internet. Thus, XRS videos are available for study, as teaching material, as a way of sharing knowledge or even sharing users' own experience in the XRS area. The latest addition to the TXRF Workgroup environment is the TXRF Blog,[17] where all type of new contributions related with "Advances in TXRF and/or X-Ray Spectrometry Science" are welcomed.

Current status

Today, we have 169 members and the number is growing even given the perceived danger of social networks! In any case, today the TXRF Workgroup enables technicians, professors, PhD students, researchers, industrialists related to XRS, engineers and scientists from more than 53 countries to interact constructively and share their knowledge and even their instrumental and technological resources at a distance.

The TXRF Workgroup is an open way for professionals with common interests to connect, allowing the development of activities where international relationships are necessary. As examples, details of the last TXRF conferences—TXRF2013 in Osaka, Japan, TXRF2015 in Denver, USA, TXRF2017 in Brescia, Italy and the next TXRF2019 in Girona, Spain—have been publicised. Recently, an intercomparative Round-Robin study proposed by Dr Alex von Bohlen from ISAS-Dortmund (Germany) was coordinated using the TXRF Workgroup as the main communication channel for the TXRF participant laboratories around the world.

Outlook

Nowadays, the TXRF Workgroup is increasingly known by the international TXRF community. It is used to share information about new conferences, journals or related papers, however, the partici-

pation of the members is still not as frequent as it should be. Therefore, the main objective for the future is that the members of the group feel free to interact with any other concerning any question, proposal or collaboration related with this field. In particular, the following activities can be proposed as goals for the TXRF Workgroup:

(1) a way to help to solve local theoretical or practical questions related to the TXRF field of any member;
(2) a way to promote the analytical strengths of TXRF and its applications at all levels;
(3) a way to open new lines of collaboration for the development of new applications of TXRF in any field of knowledge;
(4) a way to promote the development of new technological and informatics improvements for TXRF instrumentation, collaborating with potentially interested companies related to TXRF;
(5) a way to generate employment opportunities for a specialist interested in TXRF and related techniques field and its applications;
(6) a way to collaborate and/or organise inter-laboratory activities in order to standardise the application of TXRF for a great diversity of matrices according to international standards and, finally
(7) a way to do all those things that we have in mind, but are limited by the resources we have available for their development.

To conclude, the number of members and their diversity is increasing and the first steps have been taken. Looking at the growth trend and the opportunities that the future offer, the outlooks are clearly promising and, more importantly, the future will depend mainly on the TXRF Workgroup community itself. Perhaps, in the short term, the most important opportunity for the TXRF community will be the application of the European COST action ENFORCE-TXRF (CA-18130) during the next four years (2019–2023). This COST action could involve the expansion of TXRF spectrometry, which can be a unique opportunity to add TXRF spectrometry to the pool of powerful, useful and versatile modern analytical techniques for industry, research and education.

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17. TXRF Blog: http://txrfspectrometry-blog.wordpress.com

TONY DAVIES COLUMN

Can you smell smoke?

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Hafiz Abdul Azeem recently presented some interesting results from his work on atmospheric aerosols. Following their capture, he combined the optimisation of the extraction process with chromatographic separation and mass spectroscopic detection to identify various sources of pollution through their emission marker fingerprints.[1] One spin-off of this work has been the use of a specific biomarker from cellulose combustion to potentially warn of low-heat smouldering in, for example, agricultural materials in bulk storage.

Aerosols don't just come out of cans!

Atmospheric aerosols are everywhere. They are a mixture of very small particles and liquid droplets whose size means that they can be transported in the atmosphere for huge distances, changing their chemical composition as they are exposed, for example, to UV radiation and ozone during their lifetimes. You have been exposed to aerosols your whole life, and their origin (human-made or natural) affects how they interact with your body. Which molecules are observed making up such aerosols depends very much on the original source. Aerosols formed from the burning of agricultural biomass waste (or illegal slash and burn operations in rainforests!), for example, are different to those produced from motor vehicles, commercial shipping or oil-fired heating systems in buildings.

As humans, we need to be interested and aware of their presence and activity in our environment as there can be potential serious health issues. Their very small size means that they can easily gain access to our lungs. But, as a parent of twins who both had breathing difficulties at their early years, I know aerosols can be used very beneficially as a simple way to conduct very small amounts of medicines deep into the lungs of babies and small children, depositing these medicines at exactly the right locations to be most effective in re-opening the airways.[2–6]

Size is everything!

Not all aerosols make it into the lower reaches of the lungs. Our whole airway from the nose all the way down to the tiny alveolar spaces is littered with our defence mechanisms against contaminated air. These serve to clean out the contaminants in what we have breathed in before this air reaches the innermost parts of our lungs. In healthy humans, who have not destroyed these defences by, for example, smoking or working in contaminated environments for long periods, there are several different defence mechanisms targeting different sizes of contaminants. Starting with your nasal hair, and progressing to the upper respiratory tracts, the larger aerosol particles, 10 µm or larger, tend to be stopped by wall collisions. Their larger mass and fast airflow speeds mean that they don't follow the curves and bends of your airways. The heavier particles that make it past these obstacles can then be lost as gravity takes control where the airflow slows down your airway. Your defence mechanisms include traps such as small hair-like cilia, mucus and your cough reflex. Small, light aerosols can make it past your body's defences. However, if they are too small (0.5–5 µm), Brownian motion in the low-air flow in the lower regions of the lungs may mean that they stay in the airway not colliding with the walls of the lungs, just waiting to be expelled out as you exhale. Between these two extremes, aerosols containing medicines (or unwanted polluting chemicals) can make it past your defences and into the bronchus and eventually the alveoli.

Identifying aerosol origins

The ability to analyse the chemicals present in aerosols not only can deliver important information on the potential toxicity of what we are breathing, but also the distribution of these chemicals can provide important information on the origins of the aerosols.[1]

For example, phenolic compounds and sugars indicate aerosols formed from biomass burning whereas carboxylic acids and polyaromatic hydrocarbons, depending on the species identified, indicate human activity, be it motor vehicle emissions or fossil fuel use such as coal burning.

Hafiz investigated the best methods of sample preparation such as supercritical fluid extraction, liquid–liquid microextraction or hollow-fibre liquid-phase microextraction and concentrated on liquid chromatography, supercritical fluid chromatography or gas chromatography/mass spectrometry analyses (with derivatisation where necessary) for data collection and anal-

ysis leading to the identification of the individual marker substances in the aerosols. As emission marker fingerprints can be highly diverse in their chemical nature, unfortunately there is no all-in-one solution available that can be used for the detection of all of them at the same time. It requires hard-core analytical chemistry skills and access to a number of instrumental techniques for comprehensive study of various emission marker fingerprints.

It is, however, possible to suggest faster, cheaper and greener methods of analysis for certain emission markers of interest, based on their chemical nature. For example, thermal desorption hyphenated to gas chromatography/mass spectrometry can be used to study certain sugars. Handheld portable samplers are available in the market to capture aerosols on desorption tubes. These tubes can then be placed in a thermal desorption unit and analysed by online derivatisation followed by online gas chromatography/mass spectrometry analysis (Figure 1).

And this leads us back to a sugar called levoglucosan. This tracer compound has been seen as an ideal marker substance for biomass burning as the pyrolysate contains significant quantities of this sugar.

So here is the idea... the more we, as a society, are forced to move away from oil-based fuel sources the more we need to retain and store alternative sustainable biomass such a straw waste. The more we store for longer periods the greater the risk from catastrophic fires caused by undetected slow-temperature smouldering conditions in the stored material. These low-temperature, smouldering fires can occur spontaneously and can rapidly escalate to huge problems when the material is moved and exposed to fresh unlimited oxygen supplies during handling.

A challenge

So here is a challenge… as we clearly cannot deploy tens of thousands of hyphenated sample analysis gas chromatography high-vacuum mass-spectrometer laboratory analytical systems of the scale used in this method optimisation study, we need dedicated chemical-specific sensors to monitor environments such as those described above at a very low cost to supplement the failing smoke detectors. Because we need to quite urgently "smell" smouldering low-temperature fires rather than wait for the non-existent smoke to reach the smoke detectors, by which time it's probably too late! Madsen and Hafiz reported a proof of concept that aerosol signature, in the form of detection of levoglucosan evolved from smouldering fire, could be used for early detection of smouldering fire.[8] Specialised electronic noses and sensors are required for real-time detection of smouldering.

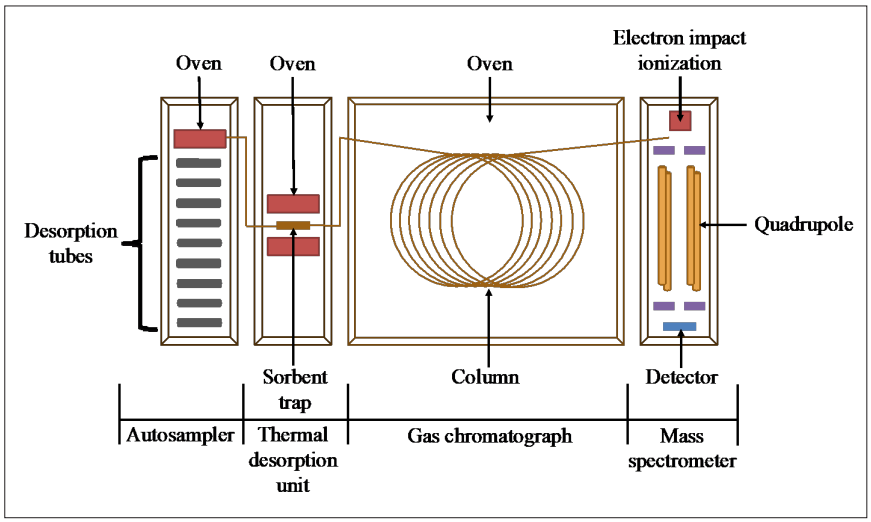

Figure 1. Illustration of various steps of thermal desorption hyphenated to gas chromatography/mass spectrometry, adapted and modified from Materic *et al.*[7]

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SAMPLING COLUMN

Sampling commitment—and what it takes...

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This column concludes the first series of Sampling Columns. More will appear in a sequel series, mainly aimed at presenting practical examples, case histories, demonstrations—all of which will assume that the value of only practicing representative sampling has been fully acknowledged and the relevant *know how* has been comprehended. Here, we end the first educational exposé of the Theory of Sampling (TOS) by focusing on the current state of awareness and with an acknowledgement of the need to involve TOS in all relevant international scientific fora, in technology, industry and in the commercial marketplace.

Historical context

The history of the World Conference of Sampling and Blending (WCSB),[1] gives a snapshot of the highly satisfactory progress seen in the last 20 years since WCSB1 (2003), in which dissemination of the Theory of Sampling (TOS) has improved greatly. Reference 2 contains a plethora of earlier relevant historical references for the interested reader.

WCSB1 was the inaugural world conference on sampling, and the proceedings were conceived as a comprehensive tribute to the founder of TOS, Pierre Gy. The historical context leading up to WCSB1 can be found in Reference 3. Among Pierre Gy's last publications is a fascinating account of the history of the development of TOS; in retrospect this is his scientific testament.[4]

Awareness

Despite this extensive activity, there are still innumerable occasions in science, technology, industry, and in governing, monitoring and regulation bodies in which awareness of the need for representative sampling is still more-or-less unknown. There are also on record cases in which this knowledge is deliberately not welcomed—we shall here a.o. focus on *why* such might be the case. Awareness and acknowledgement of the usefulness of applied TOS is an ongoing process that cannot be said to be likely to be completed anytime soon (counting in decades here). There is still much work to do.

So how to advance this critical awareness?

In areas, industrial sectors a.o., which have been "covered", this mainly scales with the intensity of additional efforts put in, but it is equally important to direct efforts to new fora in which TOS and relevant applications have not yet been introduced. This, in many ways, has been the situation for the last 10–15 years. While illuminative and inspiring presentations, lectures and workshops at yearly meetings in science, trade and industrial sectors will never fail to make a significant impact, today there is also a community which is of the persuasion that the *only thing* that counts to disseminate knowledge are webinars, LinkedIn postings and the like. History will judge which avenue fits the bill best for increasing TOS awareness. It is true, however, that systematic efforts in the electronic and the social media are only at the very beginning. The young(er) generation(s) within the TOS community will lead the way!

Minimum competence level

As part of summing up the first part of the Sampling Columns, it is advantageous to present a *brief* overview of the minimum interest and comprehension necessary to assess the scientific rationale for Theory of Sampling (TOS). Also, why TOS is the necessary-and-sufficient framework for *any* sampling task, be this the critical primary sampling or any of the subsequent sub-sampling stages along the pathway towards a representative analytical aliquot. It is emphasised that the following applies to sampling of both stationary as well as moving lots (process sampling) of all sizes, forms and shapes.

1) **All** materials and lots in science, technology and industry are *heterogeneous* (Figure 1)—not knowing about heterogeneity (or not caring to know) is a breach of due diligence for all, for OEMs, for trade companies selling sampling equipment as well as for sampling professionals. The point of departure for all sampling procedures is **heterogeneity**—and how to counteract its effect on sampling accuracy and precision.
2) The primary requirement for all sampling processes, and the corresponding equipment, is that of *counteracting* the heterogeneity met with. This is the main driving force behind all attempts to sample representatively.
3) As a minimum it is necessary to be able to distinguish between Incorrect Sampling Errors (ISE), which lead to

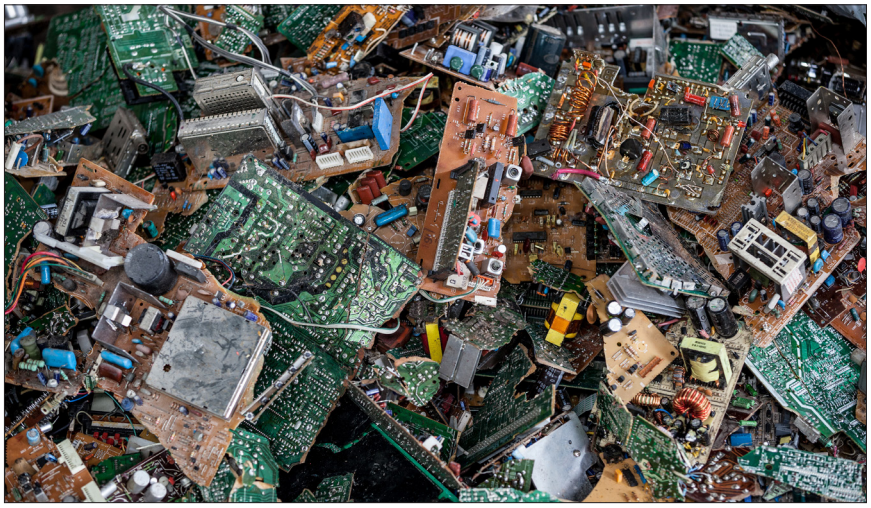

Figure 1. Heterogeneous material.

inaccurate sampling process which produces the fatal *sampling bias* and Correct Sampling Errors (CSE) which contribute to an unnecessary inflated sampling uncertainty (sampling imprecision). It is critically necessary to be able to distinguish between *analytical* accuracy and precision, and the *sampling* bias and precision. There is a world of difference, literally: while an analytical bias can be identified, quantified and thereby corrected for based on the assumption that it is constant (a fair assumption regarding analytical methods), the sampling bias cannot ever be corrected because it is **inconstant**.[5]

4) All ISE must be *eliminated* before one can get past the crippling sampling bias, after which CSE must be *minimised* in order to make the sampling process sufficiently precise (reproducible). A representative sampling process must be unbiased and with an appropriately reduced sampling imprecision so as to become "fit-for-purpose" representative.
5) TOS provides two facilities for estimating the effective magnitude of the uncertainty associated with any sampling process, i) the replication experiment[6] and ii) variographic characterisation.[7] Both of these allow identification of sampling processes as fit-for-purpose representative, or which are not in compliance with TOS (non-representative). In the latter case, TOS needs to be marshalled competently in order to remedy the sampling stations, procedures, equipment(s) identified as inferior.

These fundamental elements of TOS can be comprehended easily enough (perhaps with a little help from today's many introductory texts, at all levels imaginable, or from dedicated workshops and courses). A first level competence can in fact be established in a remarkably short time span, for the dedicated audience in as short as, say, two or three days. There are no legitimate reasons to shy away from this modicum of effort in view of the goal: full comprehension of the critical understanding needed to **never** apply a sampling process without knowing the effective level of uncertainty that can be achieved. While disregard for such a commitment would be serious enough for an individual with sampling responsibilities, picture for example an OEM selling sampling equipment and pitching sampling solutions *without* having demonstrated to the customer the true quality of the products and services offered? For true quality: read *proven* representativity.

Vade mecum

Since 2013, there has been a general standard, in effect an international standard, with the sole purpose of outlining the general principles (there are only six) and the relevant sampling unit operations (there are only four) with which to be able to address any-and-all sampling tasks—for **all** types of lots (stationary and moving lots), for **all** levels of heterogeneity (low–intermediate–high), at **all** scales and under **all** sampling conditions. TOS to the fore![8–10]

Various treatises also exist dedicated to more focused sectors, e.g. the food and feed sector. "Representative sampling for food and feed materials: a critical need for food/feed safety" is a mini-textbook, ostensibly directed towards this sector, which in reality presents the universal principles and procedures in TOS (Figure 2).[11]

It takes only a few minutes to peruse a random selection of ISO and other guiding documents before one will meet a table in which the number of increments/samples are *mandated* to be proportional to the size (weight/volume) of the lot (batch, consignment) to be sampled. Here is just one simple test of the validity of such erroneous mandates.

Figure 2. The team behind the comprehensive introduction: "Representative sampling for food and feed materials: a critical need for food/feed safety". Left-to-right: Nancy Theix, Kim H. Esbensen, Charles Ramsey, Claudia Paoletti and Claas Wagner. Photo: the author.

According to this mandate, consider two lots of the same size (for this argument assume large lots) but of radically different heterogeneity. One lot is of *very low* heterogeneity, in fact so low so as to correspond to what in many sectors is called "uniform materials" which are defined as displaying a sampling uncertainty for repeated sampling below 2 %; take a storage silo of refined sugar as an example. The other lot could, e.g., be a run-of-the-mine ore (e.g. a mineralised rock with a very large difference in the proportions of mineralisation). Clearly it

SAMPLING COLUMN

As an example of what is often considered a surprising insight for the uninitiated: It does **not** matter how large, or small, a particular lot is—the number of samples, or the number of increments to be aggregated into a composite sample in order to counteract a particular heterogeneity met with, does **not** scale with lot size, but scales with the level of material/lot heterogeneity met with.

is not logical to deploy the same number of increments/samples to counteract the empirical heterogeneity met with for these two dramatically different lots. Even if one is addressing only one-and-the-same lot (i.e. the same heterogeneity), why should small(er) lots merit a smaller number of increments/samples than considerably larger lots **if** the heterogeneity is the same throughout the lot volume? Such recommendations have not been considered in the light of TOS' full understanding of the relationships between lot/material heterogeneity and sample mass. This is a breach of due diligence, writ large!

For a compact introduction to these key issues, see References 8 and 12.

In practice…

As an example, who can condone selling "sampling equipment" and "sampling solutions" **without** having completed a replication experiment or a variographic characterisation of the unit as *installed* at the customer, with which to demonstrate the necessary "fit-for-purpose" representativity, with respect to a threshold decided upon *together* with the customer before installation? As a major example, the market and the literature is chock full of industrial hammer samplers and sampling spears (sampling thieves) that have **not** be subjected to such simple checks.

Why is this so?

This issue gets all the more interesting because there are actually a number of perfectly legitimate examples of installations of these types of sampling equipment that actually do work to a sufficient level of fit-for-purpose representativity (understandably this only is the case for *some* specific lots and materials of low heterogeneity).

In several practical cases, this has been demonstrated beyond any doubt because the *seller* was competent and conscientious enough to be in command of the simple six TOS Governing Principles (GP). Even if the *buyer* should not know this, it is still the obligation of the fair business partner in question to **insist** on performing this quality check of the equipment to be sold to the customer. This is an absolutely necessary, fair business ethics demand! This argumentation was recently laid out in full in a "tale" that has its roots in the most concrete real-world of today.[5,13]

The moral from this tale delineates the current frontline regarding **how to**, and **how much to** educate about TOS. This concerns the central question: "should one inform the customer in case he/she does not know?". There are also cases on record in which the customer manifestly does not want to know! Which is another mystery all on its own.

Most importantly: "Is **your** company, corporation, organisation, institution aware of this fundamental moral obligation?".

Is your company, corporation, organisation, institution ready to make the ultimate commitment to TOS?

To commit, or not to commit—that is the question!

What could be argument(s) against…

What *could* be arguments against being, or becoming TOS competent (enough) to live up to the above business ethical obligation? The present writer cannot conjure up **any** argument against TOS—and never mind the likely polemic accusation of being possessed by a gigantic *bias*!

This quip aside, this author has nevertheless had occasion to be exposed to a very large number of precisely such arguments during a 20-year long career within the realm of TOS. These arguments have been presented both from academic and technological communities, but especially from many sectors from industry and commerce.[14]

Consider two passionate antidotes for such unwilling, ill-informed, negative attitudes towards a commitment to invoke TOS whenever significantly heterogeneity is encountered.[15,16]

By the way, how can one ascertain whether one is addressing a lot material with a significant heterogeneity, or not (hope springs eternal…)? Easy, perform a replication experiment or a variographic characterisation.

PRACTICE, PRACTICE, PRACTICE…

Anticipating the themes that will be presented in the sequel series of Sampling Columns, dedicated to practical examples, case histories, demonstrations of both good (very good, excellent to brilliant) sampling, as well as bad (ill-informed, confused, inferior to critically dangerous) "sampling", the latter without any right to appear under such a label, examples will mainly be drawn from two sources: "Sampling—Hall of Fame" and its antithesis "Sampling—Hall of Shame".

Two more-or-less self-explanatory examples follow, one extremely simple, the other representing a much evolved and complex sampling situation.

The first is titled: "What's wrong with this sampler?" Even a cursory inspection will reveal several elements in blatant non-compliance with TOS' requirements for representative sampling (Figure 3).[17]

Figure 4 shows the principal design of a process sampling valve and PAT-sensor deployment for a complicated case in which TOS sampling from a reactor is manifestly impossible. The illustration shows a NIR PAT sensor in an optimal location for *nearly complete* sampling bias elimination and optimised sampling precision made possible by way of a "recurrent loop".[18]

The last word

This series of columns has made the strongest possible efforts to present the Theory and Practise of Sampling (TOS) as a logical set of heterogeneity-related principles and practical unit operations in an axiomatic manner. It is complete within its own restricted initiating frame-

Figure 3. Wheel of fortune? Photo: the author.

work, but it is, of course, far from complete w.r.t. a fully comprehensive theoretical foundation to which referral must be made to a series of textbooks and seminal papers, all of which constitute a logical next level for the interested reader. It is the hope that the present exposé will have served to initiate and have fostered enough interest for the reader to also want to progress towards this next goal.

It is fair to end this series with a selected key further reading list of suggestions for the next level publications (with a plethora of further references).

Further reading (a first foray selection)

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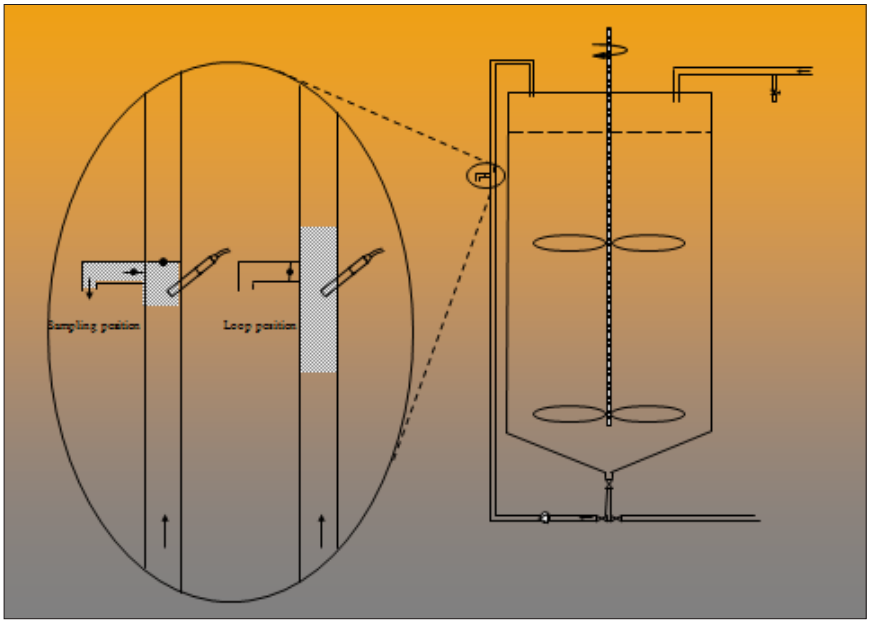

Figure 4. PAT sensor in optimal location for nearly complete sampling bias elimination and optimised sampling precision. Copyright KHE Consulting (didactic archives) reproduced with permission.

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ATOMIC

Analytik Jena enhances PlasmaQuant MS series

Analytik Jena has added features and models to its PlasmaQuant MS series. Customers will be able to configure every system in the ICP-MS series to suit their individual requirements. Further, two additional models have been introduced. The PlasmaQuant MS Q is optimised for high-throughput applications, such as quality control for consumer goods, food inspection or environmental monitoring. The PlasmaQuant MS Elite S has been developed for routine analysis of ultratrace components and is very sensitive. It is especially suitable for industries where analysis depends on the lowest detection limits and the highest recovery rates, such as applications in the semiconductor industry, quality control for high-purity chemicals or in geochemistry and geochronology.

Analytik Jena

http://link.spectroscopyeurope.com/31-010

Advion introduces the SOLATION ICP-MS analyser

Advion has released the SOLATION inductively coupled plasma mass spectrometer. It has a 90° quadrupole deflector that lowers interference by ensuring that the analyser and detector are not in line with the plasma beam, preventing neutrals and particles from entering the analyser, improving signal-to-noise and preventing contamination. The SOLATION uses triple-cone ion extraction with the sample and skimmer cones available in Ni or Pt. The third extraction cone, followed by an Einzel lens, are electrically controlled to maximise transmission of ions into the vacuum system. Dual function detectors measure in both analogue and pulse detection modes with seamless transmission between the two, to allow measurement of high and low levels in a single analysis with $>10^9$ linear dynamic range. Pulse detection captures ions generating pulses <20 ns, and is accurate and linear to a minimum dwell time of <100 µs. Analog detection is used for higher ion signals while deactivating pulse detection to extend detector lifetime.

Advion

http://link.spectroscopyeurope.com/31-003

ICP spectrometer with new torch configuration

SPECTRO Analytical Instruments has introduced the new SPECTROGREEN inductively coupled plasma optical emission spectrometry (ICP-OES) analyser, which includes a new Dual Side-On Interface (DSOI) technology. DSOI technology uses a vertical plasma torch, observed via a new direct radial-view technology. Two optical interfaces capture emitted light from both sides of the plasma, using only a single extra reflection, for added sensitivity and elimination of issues plaguing newer vertical-torch dual-view models. As a result, DSOI provides twice the sensitivity of conventional radial systems and yet avoids the complexity, drawbacks and cost of vertical dual view models.

The new instrument saves on consumables with a low-purge optic design (a UV-PLUS option offers a no-purge feature) and requires no added cooling. ORCA optical technology maximises light throughput, stability and sensitivity, and a new GigE readout system significantly boosts spectra processing and transport speeds for faster analysis speeds and shorter sample-to-sample times.

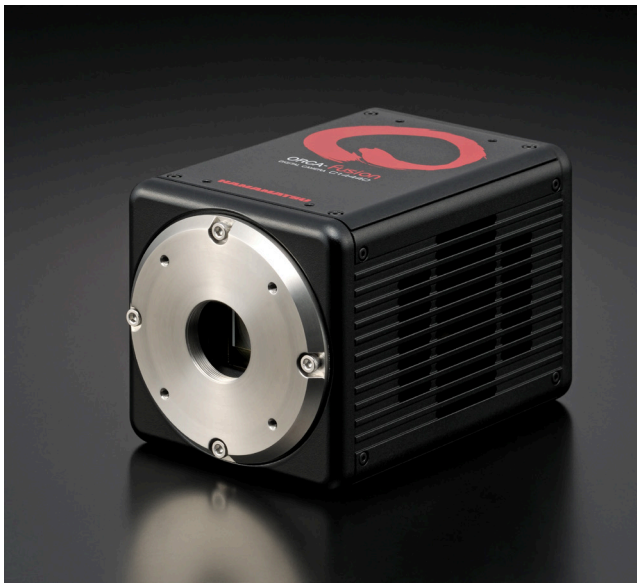
SPECTRO Analytical Instruments

http://link.spectroscopyeurope.com/31-011

NEW PRODUCTS

IMAGING

New sCMOS camera



Hamamatsu Photonics have developed a new sensor designed that combines the strengths of EMCCD and sCMOS sensors, the ORCA-Fusion. Recently, sCMOS cameras have developed into the dominant technology for imaging applications where high sensitivity and high speed are required, gradually replacing cameras based on CCD or EMCCD technology. The disadvantage of sCMOS in comparison with previous sensor technologies has always been the uniformity of the sensor in terms of gain, offset and readout noise. A broad distribution of readout noise limits the visual appearance and data quality of a camera, particularly in low-light conditions. Hamamatsu Photonics have used their experience in using offset and gain correction to improve the uniformity of sCMOS cameras and coupled this with a new sensor designed to limit noise distribution. The ORCA-Fusion is thus able to provide images and robust data at all light levels, especially in tough low-light conditions.

Hamamatsu Photonics

http://link.spectroscopyeurope.com/31-005

INFRARED

Bruker INVENIO-S research FT-IR spectrometer

Bruker has launched the INVENIO S Fourier transform infrared (FT-IR) research spectrometer that replaces the previous TENSOR spectrometer series. The INVENIO S focuses on productivity in routine and advanced laboratory analysis. Its optional Transit Channel™ allows instantaneous, software-controlled switching between measurement techniques by providing an additional, easily accessible sample compartment. The compact design allows bench space for additional, external accessories, expanding its capabilities to include IR microscopy and imaging, thermogravimetric analysis, high-throughput screening or vibrational circular dichroism. The infield upgradability to INVENIO R provides access to spectral range expansion (from far-IR to visible) and time-resolved spectroscopy (Rapid Scan, Step Scan, Interleaved TRS) when they are needed. An integrated touch panel provides intuitive guidance with typical workflows from routine to advanced applications in R&D. The INVENIO S meets all requirements of Good Laboratory Practice (GLP), and additional validation options are available.

Bruker

http://link.spectroscopyeurope.com/30-W-120

High-temperature transmission FT-IR cell

Aabspec has developed the #CXS, a new version of their #CXX transmission FT-IR cell. The #CXS keeps the features of the #CXX including ultra-low internal volume, a flow path ensuring that the reactive gases first strike the catalyst where it is exposed to the optical beam, temperatures to 800 °C etc. External surfaces are water cooled. The mounting system supplied by Aabspec with the #CXS is spectrometer specific. Temperature control is provided by the programmable Aabspec #STP-6 offering multi-ramps, multi program memory etc.

Aabspec

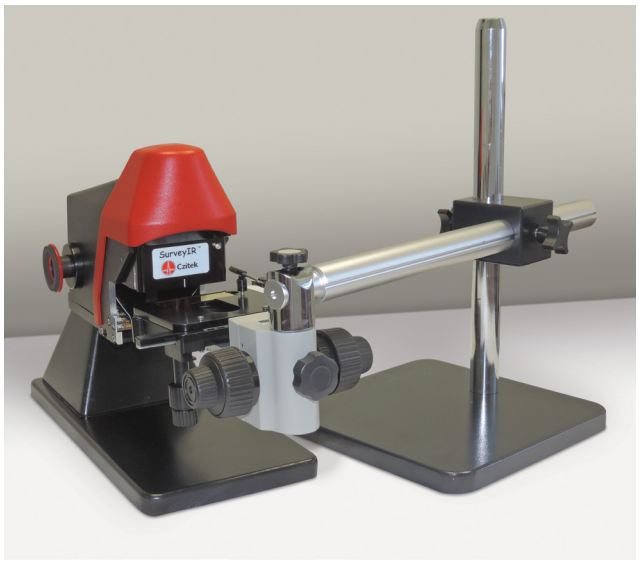
http://link.spectroscopyeurope.com/31-007

FT-IR microanalysis accessory for bulky samples

Czitek has introduced a version of their SurveyIR FT-IR microanalysis accessory for use with bulky samples, the SurveyIR$_{VS}$. The design of the SurveyIR$_{VS}$ decouples the stage from the optical microscope, allowing analysis of a large range of sample geometries along with research-grade visual images from a high-resolution colour video camera. A high depth-of-field enables rapid specimen location and manipulation in reflection and ATR viewing modes. There is good viewing quality through the diamond ATR, which simplifies target alignment and helps ensure good sample/ATR coupling including visualisation of the contact. The user can also view the sample whilst collecting data, allowing visualisation and interaction with the sample whilst observing the IR spectrum. eSpot software provides visual image display, manipulation, capture, documentation and storage. It also enables illumination mode selection and remote image mask size chosen by the user from six sample aperture options.

Czitek

http://link.spectroscopyeurope.com/30-W-119



MASS SPECTROMETRY

LC-TOF-MS system for analysis of large molecule biologicals

The pharma industry is moving towards large molecule biologicals, which are much more complex and require more sophisticated analytical tools. Waters has introduced the BioAccord™ System that can be operated by almost anyone in the lab. BioAccord is a liquid chromatography-mass spectrometry (LC-MS) instrument that uses the ACQUITY UPLC™ I-Class Plus with the ACQUITY RDa™ Detector; a small footprint time-of-flight mass spectrometer specifically developed for the BioAccord. Dedicated workflows for intact protein mass, released glycans and peptides have been developed for the system. System integration and application test is performed at the Waters factory, so the system is ready to go on installation. There are automated setup and self-diagnosis routines, and the BioAccord runs under UNIFI™, Waters' compliance-ready LC-MS informatics platform.

Waters

http://link.spectroscopyeurope.com/31-008

NIR

Crossed-cavity Czerny–Turner spectrometer

OtO Photonics' new HummingBird series are crossed-cavity Czerny–Turner spectrometers operating from 180 nm to 1100 nm. HummingBird offers the performance benefits of classic Czerny–Turner cavity designs in a smaller package of 83 × 75.5 × 26.75 mm^3 (<168 cm^3), much smaller than OtO's own SmartEngine Czerny–Turner spectrometer (~360 cm^3). Hummingbird is initially offered with a choice of two 2048-pixel sensors. OtO have designed HummingBird to take advantage of a wide range of slit and grating choices enabling optimisation of spectral bandwidth, resolution and sensitivity. Resolutions from as little as 0.2 nm FWHM can be achieved over 100 nm whilst resolution of 1.5 nm is achieved over the full 180–1100 nm operating range. Communication with the spectrometer is via high speed (480 Mbps) USB2.0 or six user-programmable digital I/Os. SpectraSmart software enables setup within minutes, and there is a Software Developer Kit for Windows and example code for Linux to integrate into a broad range of industrial, medical, pharmaceutical and environmental applications.

AP Technologies

http://link.spectroscopyeurope.com/31-006

Fibre optic multiplexer for NIR spectrometers

Galaxy Scientific has introduced a fibre optic multiplexer for use with NIR spectrometers, which allows a single spectrometer to automatically switch between up to ten different sampling devices. This enables NIR measurements from multiple sampling points or multiple product streams. It is designed to accept standard SMA905 low-OH optical fibre inputs (commonly used for connecting a NIR spectrometer to a process probe) and is designed to switch 600 µm solid core fibre. Smaller core fibre or larger core fibre bundles are also compatible. The multiplexer is factory configurable at the time of order to have any number of channels between 2 and 10 and more channels can be added

NEW PRODUCTS

after purchase. The unit can be placed close to the sample points and distant from the spectrometer, reducing the cost of long fibre optic runs while still protecting sensitive instrumentation.
Galaxy Scientific
http://link.spectroscopyeurope.com/31-004

New fNIR optical imaging systems

BIOPAC Systems, the global distributor for fNIR Devices, has announced the latest generation of their functional near infrared (fNIR) optical imaging systems. The new high-density imaging systems provide in-lab or real-world cognitive function assessments for physiology researchers looking to understand brain activity without fMRI. The extra-lightweight sensor fits comfortably on the forehead where it monitors relative changes in oxy or deoxy haemoglobin as a proxy for the brain activity in the prefrontal cortex.

The new fNIR systems are available in three versions. The fNIR 2000C is a stationary unit that collects data from up to 18 optodes. The fNIR 2000M is a wireless and mobile imager that collects data from up to 18 optodes and can be used while subjects are performing tasks in the lab or in the real world. The fNIR 2000S is a 54-optode capable imager with advanced features for recording up to three subjects simultaneously. A new through-the-hair sensor will allow researchers to assess other areas of the brain such as motor and visual cortices. Adding in different parts of the brain increases understanding of brain activity without the complications of fMRI.

All systems include fNIRSoft and COBI software for data collection and analysis. Data can be synchronised with and imported into AcqKnowledge Software to understand the physiological response, including EEG, EDA, ECG, BP and other important physiology signals.
BIOPAC Systems
http://link.spectroscopyeurope.com/31-002

PHOTONICS AND OPTICS

UV-NIR neutral density filters

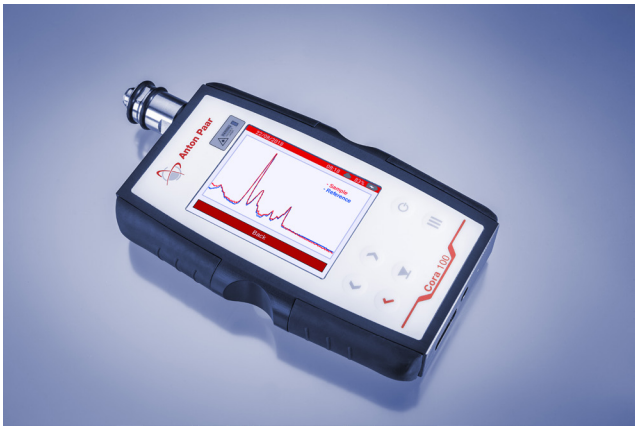
Acton Optics & Coatings has introduced a new series of UV-NIR neutral density filters. Thanks to patented UV coating processes, these can include broadband UV-NIR neutral density filter performance down to 190 nm. The new ND filters, which are suitable for use with broadband sources like xenon, deuterium and tungsten halogen, have been designed to optimise the utility of precision optical systems, spectrometers and medical systems.

Various standard densities are available from 0.3 OD to 2.5 OD and the new filters can be stacked to create additional or deeper densities. The exclusive filter coatings can also be deposited on custom-sized substrates for OEM applications and, if required, can be designed for other optical density values.
Acton Optics & Coatings
http://link.spectroscopyeurope.com/31-001

RAMAN

Cora 100 handheld Raman spectrometer from Anton Paar

Anton Paar has introduced the Cora 100 handheld Raman spectrometer for on-the-spot identification of explosives, narcotics and hazardous materials. The intuitive software and accessories can be used by anyone, without formal training in Raman spectroscopy. The small footprint (16 × 10 × 3 cm), small weight (700 g) and rugged construction make it suited to single-handed operation and on-site identification of substances. The Raman analyser has successfully been tested according to military specifications, MIL-STD 810G, as well as European tests for dust and water, and is classified as IP67 waterproof. Spectral libraries for narcotics, hazardous materials, explosives and chemical warfare agents are available. Customised libraries can also be created by the user. The collected data is saved and stored in the spectrometer for further report generation. The point-and-shoot adapter is suited for measurements through bottles or plastic bags for identifying liquids and powders. Quick non-contact analysis without moving samples, for example potential explosives, can be performed with the right-angle sampling adapter.
Anton Paar
http://link.spectroscopyeurope.com/30-W-118



Conferences 2019

9 April, London, United Kingdom. **Advances in Hyphenated Mass Spectrometry.** mark_mcdowall@icloud.com, https://www.bmss.org.uk/advances-in-hyphenated-mass-spectrometry/.

15–18 April, Sao Paulo, Brazil. **XII Workshop on Sample Preparation (XII WPA).** http://www.iq.usp.br/wpa2019/.

17–18 April, Osaka, Japan. **9th International Conference and Exhibition on Spectroscopy and Analytical Techniques.** lcms2018hk@gmail.com, https://spectroscopyconference.massspectra.com/.

30 April–2 May, Chester, United Kingdom. **APACT19.** https://apact.co.uk/.

1 May, Sheffield, United Kingdom. **The Sixth Mass Spectrometry Imaging One Day Meeting.** Dr Jamie Young, jamie.young@shu.ac.uk, https://www.eventbrite.com/e/bmss-sig-imaging-symposium-2019-tickets-51956350844.

5–10 May, San Jose, United States. **Conference on Lasers and Electro-Optics (CLEO).** confserv@osa.org, https://www.cleoconference.org/home/.

6–9 May, Beijing, China. **The 9th World Conference on Sampling and Blending-WCSB9.** http://www.wcsb9.com/.

13–15 May, Edinburgh, United Kingdom. **Challenges in Analysis of Complex Natural Mixtures: Faraday Discussion.** http://www.rsc.org/events/detail/29574/challenges-in-analysis-of-complex-natural-mixtures-faraday-discussion.

15–16 May, Wageningen, Netherlands. **Boosting Innovation in Food and Agriculture.** http://www.fanext.com/.

20–24 May, Vienna, Austria. **15th International Symposium on Isotope Hydrology.** Olive Kracht, o.kracht@iaea.org, https://www.iaea.org/events/international-symposium-on-isotope-hydrology-2019.

20–21 May, Vancouver, Canada. **International Conference on Hyperspectral Imaging and Remote Sensing (ICHIRS 2019).** https://waset.org/conference/2019/05/vancouver/ICHIRS.

20–21 May, Zurich, Switzerland. **21st Annual European Pharma Congress.** pharmaeurope@pharmaceutical-conferences.org, https://www.ideaconnection.com/conferences/3879-21st-Annual-European-Pharma-Congress.html.

22–23 May, Rotterdam, Netherlands. **The 3rd International Conference and Exhibition on Petrochemical and Oil Analysis (PEFTEC 2019).** info@ilmexhibitions.com, https://www.ilmexhibitions.com/peftec/.

22–24 May, Berlin, Germany. **2nd International Symposium on Single Photon Based Quantum Technologies.** Kerstin Wicht, events@picoquant.com, http://www.quantum-symposium.org.

26–30 May, Helsinki, Finland. **SETAC Europe 26th Annual Meeting.** setac@setaceu.org.

30 May–1 June, Jena, Germany. **Bunsentagung 2019: 118th General Assembly of the German Bunsen Society for Physical Chemistry.** https://veranstaltungen.gdch.de/tms/frontend/index.cfm?l=8502&modus=.

2–6 June, Atlanta, Georgia, United States. **67th ASMS Conference on Mass Spectrometry.** office@asms.org, https://www.asms.org/conferences/annual-conference.

2–5 June, Nara, Japan. **15th International Symposium on Applied Bioinorganic Chemistry (ISABC 15).** http://web.apollon.nta.co.jp/isabc15/.

9–14 June, Mexico City, Mexico. **Colloquium Spectroscopicum Internationale XLI (CSI XLI).** info@csi2019.mexico.com, http://www.csi2019mexico.com/.

11–12 June, Muenster, Germany. **5th International Workshop on Electrochemistry/Mass Spectrometry (ElCheMS 2019).** martin.vogel@uni-muenster.de, https://www.uni-muenster.de/Chemie.ac/en/karst/workshops/elchems.html.

16–20 June, Split, Croatia. **5th International Sclerochronology Conference (ISC2019).** Melita Peharda, isc2019@izor.hr, http://jadran.izor.hr/isc2019/index.html.

17–20 June, Oslo, Norway. **16th Scandinavian Symposium on Chemometrics (SSC16).** ssc16@nofima.no, http://ssc16.org/.

17–19 June, London, United Kingdom. **4th International Congress on Organic Chemistry and Advanced Drug Research.** https://organicchemistry.pulsusconference.com/.

23–27 June, Munich, Germany. **Laser World of Photonics Congress.** Ellen Richter-Maierhofer, info@photonics-congress.com, https://www.photonics-congress.com/about/conferences/index.html.

25 June, Oxford, United Kingdom. **RamanFest 2019: Conference on Advanced Applied Raman Spectroscopy.** ramanfest.uk@horiba.com, http://www.ramanfest.org/.

25–28 June, Dorval, Quebec, Canada. **Spectr'Atom 2019.** Diane Beauchemin, diane.beauchemin@chem.queensu.ca, http://www.csass.org/SpectrAtom2019.html.

25–28 June, Dorval, Canada. **63rd International Conference on Analytical Sciences and Spectroscopy (ICASS).** Diane Beauchemin, diane.beauchemin@chem.queensu.ca, http://www.csass.org/ICASS.html.

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27–29 June, Amsterdam, Netherlands. **18th Annual Congress on Pharmaceutics & Drug Delivery Systems.** clarajane567@gmail.com, https://pharmaceutics.annualcongress.com/.

30 June–3 July, Warsaw, Poland. **7th International Symposium on Metallomics.** Ryszard Lobinski, sekretariat@metallomics2019.pl, http://metallomics2019.pl/.

8–12 July, Auckland, New Zealand. **International Conference on Advanced Vibrational Spectroscopy (ICAVS10).** ICAVS Secretariat, Podium Conference Specialists, 2661 Queenswood Drive, Victoria, BC, Canada, V8N 1X6. http://www.icavs.org/2019-conference/.

25–26 July, Rome, Italy. **3rd European Congress on Pharma and Pharmaceutical Science.** https://european-pharma.pulsusconference.com/.

28 July–2 August, Yokohama, Japan. **International Geoscience and Remote Sensing Symposium (IGARSS 2019).** https://igarss2019.org/.

5–9 August, Lombard, IL, United States. **68th Annual Denver X-ray Conference (DXC 2019).** http://www.dxcicdd.com.

5–9 August, Ephesus, Kusadasi, Aydin, Turkey. **4th International Turkish Congress on Molecular Spectroscopy (TURCMOS 2019).** Pinar Tekbas Çam, info@leoncongress.com, http://turcmos.com/.

18–23 August, Barcelona, Spain. **Goldschmidt 2019.** https://goldschmidt.info/2019/.

25–30 August, Berlin, Germany. **21st International Society of Magnetic Resonance (ISMAR) Conference joint with EUROISMAR 2019.** euroismar2019@fmp-berlin.de, https://conference.euroismar2019.org/event/1/.

1–5 September, Istanbul, Turkey. **Euroanalysis XX.** Alen Demirel, alen.demirel@brosgroup.net, http://euroanalysis2019.com/.

3–5 September, Manchester, United Kingdom. **40th BMSS Annual Meeting 2019.** bmssadmin@btinternet.com, https://www.bmss.org.uk/bmss-annual-meeting-2019/.

8–13 September, Maui, Hawaii, United States. **15th International Conference on Laser Ablation (COLA 2019).** Vassila Zorba, vzorba@lbl.gov, https://cola2017.sciencesconf.org/resource/page/id/11.

15–20 September, Gold Coast, Australia. **NIR-2019.** nir2019@yrd.com.au, http://www.nir2019.com/.

23–26 September, Freiberg, Germany. **Colloquium Analytical Atomic Spectroscopy 2019 (CANAS 2019).** canas@chemie.tu-freiberg.de, https://tu-freiberg.de/canas.

24–26 September, Amsterdam, Netherlands. **10th Workshop on Hyperspectral Image and Signal Processing: Evolution in Remote Sensing (WHISPERS).** http://www.ieee-whispers.com.

13–18 October, Palm Springs, United States. **SciX 2019 Conference (formerly FACSS): Annual National Meeting of Society for Applied Spectroscopy (SAS)/The 46th Annual North American Meeting of the Federation of Analytical Chemistry and Spectroscopy Societies..** scix@scixconference.org, http://www.scixconference.org.

5–8 November, Prague, Czech Republic. **9th International Symposium on Recent Advances in Food Analysis (RAFA 2019).** jana.hajslova@vscht.cz, http://www.rafa2019.eu/.

Courses 2019

11–15 March, Gembloux, Belgium. **Training on Vibrational Spectroscopy and Chemometrics.** Juan Antonio Fernández, j.fernandez@cra.wallonie.be, http://www.cra.wallonie.be/en/annual-spectroscopy-and-chemometrics-training.

29 April, Chester, United Kingdom. **APACT19 Pre-Conference Courses.** https://apact.co.uk/pre-conference-courses.

24–27 June, Lille, France. **Interpretation of Infrared and Raman Spectra.** https://www.ircourses.org

13–20 September, Dresden, Germany. **5th International Summer School Spectroelectrochemistry.** https://www.ifw-dresden.de/news-events/scientific-events/summer-school-spectroelectrochemistry/.

Exhibitions 2019

12–14 March, Dubai, United Arab Emirates. **ARABLAB 2019.** info@arablab.com, https://www.arablab.com/.

17–21 March, Philadelphia, United States. **69th Pittcon 2019: Conference on Analytical Chemistry and Applied Spectroscopy.** pittconinfo@pittcon.org, https://pittcon.org/.

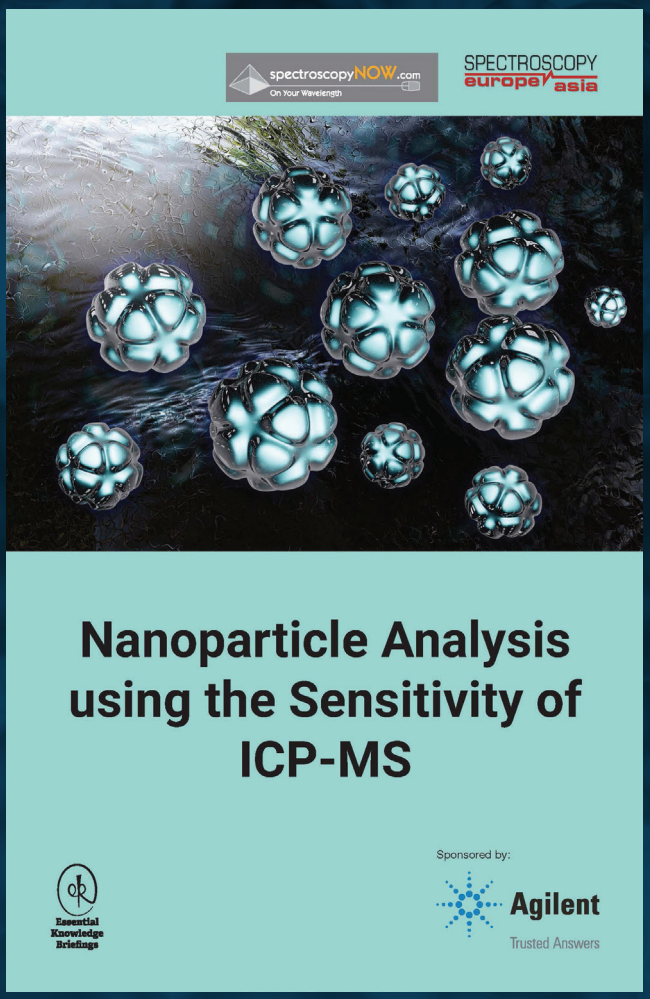
20–22 March, Shanghai, China. **Laser World of Photonics China 2019.** info@world-of-photonics-china.com, https://world-of-photonics-china.com.

7–9 May, Beijing, China. **AchemAsia 2019.** https://www.achemasia.de.

26–27 June, Basel, Switzerland. **Chemspec Europe 2019: 34th International Exhibition for Fine and Speciality Chemicals.** https://www.chemspeceurope.com/.

9–11 July, Johannesburg, South Africa. **Analytica Lab Africa.** Barbara Kals, barbara.kals@messe-muenchen.de, https://www.analytica-africa.com/.

24–26 September, Amsterdam, Netherlands. **Spectro Expo 2019.** http://www.spectroexpo.com.



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