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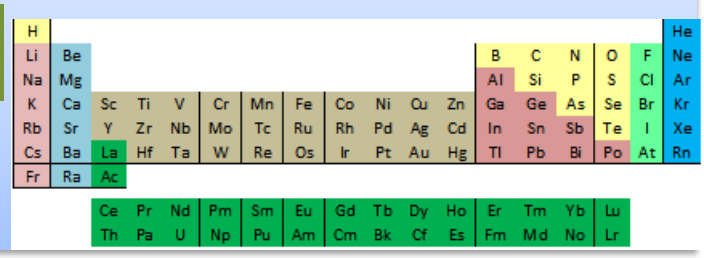

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Canadian Society
for Analytical Sciences and Spectroscopy

President's MESSAGE

Dr. Diane Beauchemin

December 28, 2019

Dear members,

Thank you for being part of CSASS, which would not survive without you. With only 83 active members currently, your help would be appreciated to grow CSASS. Could you convince one acquaintance to join? Do you have any suggestion on how to attract new members? The new free job posting initiative is one such attempt. Are you looking for a new employee, post-doctoral fellow, or graduate student? Every CSASS member in good standing can have their vacancy posted on the CSASS web site free of charge. Simply e-mail me your advertisement and I will get it posted.

As it stands, most members join/re-join as part of the International Conference on Analytical Sciences and Spectroscopy (ICASS), which is why it should be held annually. I have been involved in its organization for many years and would not mind to pass on the torch. Would any of you be interested in organizing ICASS in the future? I would be happy to share my experience. Although it involves a lot of work, it is rewarding to see people come together and enjoy the relaxing format (40-min coffee breaks, 1.5–h lunch) and numerous networking activities (see the Mark Your Calendar page in this newsletter).

Please do not hesitate to share your thoughts with me, which will be anonymously shared with the National Executive Committee (unless you specifically request to be identified). After being dormant for several years, CSASS is coming alive again. Let's work together to make it thrive.

With best wishes of health and happiness in 2020,

Diane Beauchemin
CSASS President
diane.beauchemin@queensu.ca

Happy New Year!

More ... Highlights

ICASS 2019

Burgener Research Graduate Student Travel Award Presentation

DEVELOPING THE CONTINUOUS ON-LINE LEACHING METHOD FOR USE IN BIOACCESSIBILITY RISK ASSESSMENTS OF CONTAMINATED SOILS WITH INDUCTIVELY COUPLED PLASMA MASS SPECTROMETRY

Alastair Kierulf*, Iris Koch†, and Diane Beauchemin*; *Queen's University, Kingston, ON;
†Royal Military College of Canada, Kingston, ON

Soil is arguably the most important natural element not found on the periodic table. Used in agriculture, industry, and in our environment, soil provides numerous benefits to Canadians. However, these benefits can quickly become dangerous when soil is contaminated.

Ph. D. student Alastair Kierulf (right) and ICASS Chair Diane Beauchemin (left) on behalf of Burgener Research

Contaminated soils have a direct effect on humans as many (usually unknowingly) incidentally ingest soil every day. Ingestion gives a worst-case-scenario of exposure as it has the highest likelihood that toxic contaminants will enter the bloodstream. To investigate the amount and effects of a toxin entering the bloodstream, the most accurate method is a bioavailability study. Bioavailability is the amount of a toxin that is present in the bloodstream and its effects on target organs. Bioavailability studies are expensive, time consuming, and require animal subjects [1]. A simpler method is a bioaccessibility study, which looks at the amount of a toxin that is made available for absorption into the bloodstream during digestion using artificial gastrointestinal matrices. Bioaccessibility studies are faster, cheaper, and still give an indication of the maximum possible bioavailable fraction.

The recent United States Environmental Protection Agency bioaccessibility method [2] utilizes a batch method of matrix leaching whereby soil is soaked in artificial gastric juice for 1 hour at 37 °C to most closely reflect the conditions of the human digestive system. Some drawbacks of this method are that it only uses gastric juice (omitting the valuable bioaccessibility information obtained from the saliva and intestinal matrices), and there is no kinetic information obtained during the leaching process. The continuous on-line leaching method offers improvements to this batch method of bioaccessibility analysis. The continuous on-line leaching method has been applied to bioaccessibility studies on rice, corn bran, bread, wheat and fish [3-7].

Burgener Research Graduate Student Travel Award Presentation (continued)

This method has each artificial gastrointestinal matrix sequentially pumped through a mini-column containing the sample and sent directly to the detector. Conditions in this method reflect the worst-case scenario of elevated gastric acidity, a temperature of 37 ℃, and a maximal release of toxic elements. Leaching time is significantly less than in the batch method as results for all three gastrointestinal matrices are obtained in only 25 minutes, instead of over 4 hours with the batch method. While this method has been applied to many different samples, it has not been directly standardized or validated against an accredited method. Consequently, there is no consensus on certain parameters such as sample size or column volume. For example, the study on rice used a sample of 0.2 g while the studies on corn, bran, bread, wheat, and fish used 0.1 g, 0.25 g, 0.4 g, and 0.1 g of sample, respectively [3-7]. The authors of the wheat study also noted that a larger mini-column volume improved reproducibility [6]. It is therefore imperative to find optimal analysis parameters in order to validate the on-line method against the other established bioaccessibility methods.

Since there is a wide variability in sample size reported in the literature, this was the first parameter investigated. Mini-columns were made using a 6 cm long, 0.79 cm outer diameter, 0.63 cm inner diameter polytetrafluoroethylene (PTFE) tube. Certified contaminated soil "TILL-4" from the Canadian Certified Reference Materials Project was selected for elemental analysis of As, Cr, Pb, and Sr. Soil samples of 0.2 g, 0.4 g, 0.6 g, and 0.8 g were wrapped in dry, saliva-soaked glass wool and placed into the PTFE tube, using a small 'plug' of wool at each end to secure it. Another set of mini-columns were prepared by measuring 0.5 g of soil directly into the PTFE tube, using a small 'plug' of wool at each end to secure it. Another set of mini-columns were prepared by measuring 0.5 g of soil directly into the tube (not wrapped in wool) and plugged at each end. Analysis was performed similar to previous studies [6] using a Varian 820 MS inductively coupled plasma mass spectrometer (ICPMS) with Burgener T2100 nebulizer and Scott double-pass spray chamber. A collision-reaction interface was also used to mitigate interferences. Data was acquired in time resolved mode, where the counts-per-second signal for each mass-to-charge ratio was measured as a function of time.

For all sample sizes, the gastric phase leached the majority of elements. This is likely due to the high acidity of the gastric phase. The smaller sample sizes of 0.2 g and 0.4 g had some leaching in the saliva and intestinal phases. The column with just 0.5 g of soil (not wrapped in glass wool) was plagued with back-pressure issues and an atypical flow injection profile. Because of this, more analyte was observed in the residual phase for the 0.5 g samples and indicates that there was incomplete leaching of those samples. Omitting the glass wool step also did not reduce sample loss during the mini-column preparation (based on weigh-by-difference sample recovery calculations).

In order to validate the continuous on-line leaching method against other bioaccessibility methods, a defined set of parameters must be empirically determined. Future work will use this sample size analysis when validating the on-line method to ultimately help the continuous online leaching method become a trusted method for bioaccessibility analysis in the future.

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More ... Highlights

ICASS 2019

Thermo Fisher Scientific Spectroscopy Award

ATOMICALLY PRECISE CLUSTERS: EXCITED STATE PROPERTIES AND GIANT TWO-PHOTON ABSORBANCE

Dr. Kevin Stamplecoskie, Queen's University, Kingston, ON, Canada

Nanomaterials synthesis has been reaching new levels of precision. It is now possible to synthesize metal and semiconductor particles with exact atomic composition. These atomically precise nanomaterials are referred to as "clusters". The Stamplecoskie group has recently contributed significantly to the synthesis of gold and silver clusters, and to the spectroscopy characterization; leading to a deeper fundamental understanding of this emerging materials.

The isolation of atomically precise clusters (eg. thiol protected silver clusters like Ag18SR14) present significant synthetic challenges. Particularly challenging is control over the reduction steps, which is critical in isolating clusters with high purity. The Stamplecoskie group has used a photoinitiator, previously exploited for the synthesis of larger nanoparticles, to synthesize Au25(glutathione)18 clusters with higher purity and yield than other synthetic methods. The advantages of this photochemical method were further realized in the isolating Ag18(glutathione)14 for the first time. This silver cluster has numerous advantageous properties for biomedical imaging and cancer therapy!

Clusters exhibit unique optical properties including long-lived excited states, complex excited state dynamics, and tuneable photocatalytic activity. Tuning the optical properties of clusters is crucial to realizing their potential as a photonic material. Femtosecond pump/probe spectroscopy studies were used to elucidate the excited state properties of clusters. Included herein were a series of 4 Au25 and 3 Au18 clusters. A model that includes a manifold of excited states has been proposed by Stamplecoskie that describes their complex behaviour following light excitation. Importantly, the model offers an understanding of the different fluorescent quantum yield of this series of gold clusters as well as the anomalously large solvent dependence on emission quantum yields observed for some thiol protected gold species. These studies, and the excited state model, will be important to the discovery of optimal clusters for photocatalysis as opposed to those most advantageous for biomedical applications.

Dr. Kevin Stamplecoskie (Winner, right) and Michel Alsayegh (Thermo Fisher Scientific representative, left)

Thermo Fisher Scientific Spectroscopy Award (continued)

Lastly, pump/probe spectroscopy was used to investigate the two-photon absorbance of more than a dozen gold and silver clusters. Several clusters have been reported to exhibit "giant" two-photon cross section, making them able to absorb non-linear excitation with unprecedented cross sections. These large non-linear effects make clusters excellent candidates for next generation biomedical imaging (and possibly photodynamic therapy). Polarizability, and anisotropic in molecular structure have been previously highlighted as features to enhance non-linear absorption. However, our studies show that a double resonance effect is the most critical factor to achieving high cross sections for two-photon absorption. Furthermore, due to this double resonance requirement, in biomedical imaging it is absolutely necessary to match the molecular contrast agent (clusters) with the laser excitation wavelength. In other words, it is as important to consider the choice of laser as it is to use the optimal cluster for achieving maximal signal and contrast in two-photon imaging.

Overall the Stamplecoskie group aims to synthesize new gold and silver clusters as the next generation of photonic materials. Steady-state and ultrafast spectroscopy techniques are used to push the limits of fundamental knowledge of these emerging materials, and to design new clusters with enhance optical properties.

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Invitation to contribute to the CSASS Newsletter

Do you have information that could be of interest to other CSASS members? Examples include a description of your company or research activities, useful tricks that save valuable time, historical notes about CSASS, and news that you would like to share.

If so, please e-mail the information to the CSASS Editor, Liyan Xing (lyxing2002@hotmail.com) by March 31.

Mark Your Calendar

64th International Conference and Analytical Sciences and Spectroscopy **(64th ICASS)**

August 10-12, 2020

Ambassador Hotel and Conference Centre

1550 Princess Street, Kingston, Ontario K7M 9E3, Canada

The registration includes:

- ✓ **All meals;**
- ✓ **A tour of Kingston on August 10;**
- ✓ **A 3-hour sunset dinner cruise of the Thousand Island on a triple deck Mississippi paddle – wheeler (picture on upper right) on August 10.**
- ✓ **Banquet at the Ambassador Hotel (see picture on the lower right) on August 11.**

The early bird deadline is May 31.

See http://www.csass.org/ICASS.html for details

Invitation to contribute to the 64th ICASS

So far, the list of sessions is as follows:

- Agricultural and food safety – Alastair Kierulf and Diane Beauchemin (Queen's University, Kingston, ON)
- Environmental analysis – Eve Kroukamp (PerkinElmer, Woodbridge, ON)
- Forensic analysis – Margaret MacConnachie and Diane Beauchemin (Queen's University, Kingston, ON)
- Industrial applications – Robert Teuma-Castelletti and Diane Beauchemin (Queen's University, Kingston, ON)
- Innovations from manufacturers – Diane Beauchemin (Queen's University, Kingston, ON)
- Electrochemical and surface analysis – Zhe She (Queen's University, Kingston, ON)
- Nanomaterials and their analysis – Ram Lamsal and Diane Beauchemin (Queen's University, Kingston, ON)
- NMR – Gang Wu (Queen's University, Kingston, ON)
- Sample introduction systems for the inductively coupled plasma – Ahmed Al Hejami and Diane Beauchemin (Queen's University, Kingston, ON)
- Separations/Mass spectrometry – Karen Waldron (Université de Montréal, Montréal, QC)
- Spectroscopy of Emerging Photonic Materials – Kevin Stamplecoskie (Queen's University, Kingston, ON)

Is there a topic dear to your heart that is missing from the above list? If so, please step forward to **organize a symposium** in exchange for a **25% discount on the registration fee** per half-day session that you organize.

Would you like to **offer a day-long course** immediately after ICASS on August 13 in exchange for a **complimentary ICASS registration**? So far, only the following courses are contemplated:

- Single particle ICPMS (Diane Beauchemin, Queen's University)
- Risk assessment (Iris Koch, RMC).

Please contact the ICASS Chair, Diane Beauchemin (diane.beauchemin@queensu.ca) as soon as possible.