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WELCOME TO THE 53RD ICASS

Dear colleagues:

On behalf of the ICASS 2007 organizing committee, it is my great pleasure to welcome you to the 53rd International Conference on Analytical Sciences and Spectroscopy at Trent University.

This conference is a Canadian Society for Analytical Sciences and Spectroscopy (CSASS) sponsored event and continues the tradition of previous ICASS meetings providing a venue for analytically oriented scientists to share their latest discoveries with an international audience. The 2007 program covers topics from general analytical chemistry over molecular spectroscopy to many flavours of mass spectrometry and various applications in environmental research.

As a first for ICASS, we will conclude the meeting with a post-symposium dedicated to multicollector ICP/MS. This year's meeting will also pick up a previous tradition of joining forces with the Canadian Thermal Analysis Society, which organized a full concurrent CTAS program.



Needless to say that a conference of this magnitude would not be possible without all the volunteers, who helped with the organization and are still involved in running this exciting event as you read these lines. In particular, I would like to single out Dr. Delphine Foucher, who kept everything on track and was the real organizer behind the scenes. I would also like to take this opportunity to thank all of our sponsors and exhibitors, who contributed to the meeting in many different ways.

In closing, I wish you all a delightful and productive conference. I hope you will enjoy many fruitful discussions, either during the technical program, the Trent Canal Boat Cruise on Tuesday afternoon or one of the other social events.

Once again, welcome to Trent!

Holger Hintelmann
ICASS 2007 Conference Chair



CANADIAN THERMAL ANALYSIS SOCIETY

AN AFFILIATE OF THE NORTH AMERICAN THERMAL ANALYSIS SOCIETY

www.CTAS.org

Dear ICASS-CTAS Participants,

It is my great pleasure to welcome you all at the 2007 ICASS-CTAS joint conference in Trent University, Peterborough, organized by the Canadian Society for Analytical Sciences and Spectroscopy (CSASS) and Canadian Thermal Analysis Society (CTAS). CSASS and CTAS both are sisterly organizations. Generally, most of the years, the International Conference on Analytical Sciences and Spectroscopy (ICASS) and CTAS annual conferences are organized by CSASS and CTAS separately. However, every now and then, these two organizations bond together to organize ICASS-CTAS joint conferences. This is one of such event. As a member of both the societies, I feel excited when they conjoin since I truly believe that 'in unity lies the strength'.

You're cordially invited to attend any session at your convenience regardless of your affiliation to the specific society. The three-day CTAS section consists of a one-day training session and vendor presentation, a two-day technical session with oral and poster presentations and a three-day instrument exhibition. To recognize the contribution of students, a Student Award of \$200 will be presented to the student who makes the best poster and/or oral presentation at the CTAS session.

It is also my great pleasure to inform you that there'll be a special chapter of the Journal of Thermal Analysis and Calorimetry (JTAC) dedicated to the CTAS for the selected 12 papers, presented in CTAS session. The papers will be accepted on first come first serve basis and full papers will be published only after a positive review in the JTAC special issue.



If you have not submitted yet, please submit your paper (8 pages maximum) as soon as possible to me at scmojumdar@hotmail.com

I hope you will truly enjoy the social programs and explore the unique natural beauty of Peterborough as well as of our great country Canada. I would also like to extend a warm and cordial invitation to all of you to attend the future CTAS and/or ICASS-CTAS conferences. I also want to take this opportunity to thank Dr. Holger Hintelmann and his team for their hard work towards making this great event a success.

Yours truly,

Subhash C. Mojumdar, Ph.D.
CTAS Program Chair
University of Waterloo



Canadian Society for Analytical Sciences and Spectroscopy

Dear Colleagues:

It is my pleasure, on behalf of the Canadian Society for Analytical Sciences and Spectroscopy (CSASS) National Executive Committee, to welcome you to the 53rd International Conference on Analytical Sciences and Spectroscopy (ICASS) at Trent University, Peterborough. ICASS is an annual conference to provide international spectroscopists and analytical chemists a forum for the dissemination of new scientific and technical knowledge and exciting networking opportunities.

CSASS has members from across Canada and from many other countries. Local sections exist in Vancouver/Victoria, BC Interior, Edmonton/Alberta, Southern Ontario, Ottawa, the Province of Quebec, and Northern Ontario (new section in 2006). Each of these sections organizes events such as local tours, workshops, guest lectures, and symposia. If you are interested in participating in the local section please contact the section chair or director (see <http://www.csass.org> for a list of all NEC members).

CSASS also sponsors an internationally recognized, peer reviewed journal – the Canadian Journal of Analytical Sciences and Spectroscopy (CJASS). This journal has recently become available electronically at <http://www.cjass.ca>, and is available to all CSASS members as part of their membership fee. Your publication to CJASS can now be submitted online!

I would like to thank Dr. Holger Hintelmann, the conference chair, and his organizing committee for all of the work that they have done in putting together this conference. It takes a great deal of time and commitment to produce such a successful technical program. I would also like to thank all of the exhibitors and sponsors who have contributed to ICASS 2007, without whose generous support it would not have been possible to run this conference. Please take the time to visit these companies to personally show your appreciation.

Thank you for attending ICASS 2007, and I hope that you enjoy the conference from both a technical and social aspect.

Sincerely,
Teresa Switzer
CSASS President



Société Canadienne des Sciences Analytiques et de Spectroscopie

Chers Collègues:

Il me fait grand plaisir de vous souhaiter, au nom du Comité Exécutif National de la Société Canadienne de Spectroscopie et des Sciences Analytiques, un cordial bienvenue à la 53^e Conférence Internationale des Sciences Analytique et de Spectroscopie (ICASS), ici à l'université Trent de Peterborough. Cette conférence annuelle est un lieu de rencontre international des spectroscopistes et des chimistes analystes où se propagent à la fois de nouvelles connaissances scientifiques et techniques et des opportunités d'échange stimulantes.

Notre Société regroupe des membres à travers le Canada et de nombreux autres pays. Des sections locales existent à Vancouver/Victoria, en CB Intérieure, à Edmonton/Alberta, au Sud de l'Ontario, à Ottawa, au Québec, et (depuis 2006) au Nord de l'Ontario. Chacune de ces sections organise des activités comme des visites guidées, des ateliers, des conférences locales et des symposiums. Si vous êtes intéressé à participer à l'une de ces sections locales, vous êtes prié de contacter le président de section ou le directeur (voir <http://www.csass.org> pour une liste de tous les membres).

La société commandite aussi un journal avec comité de lecture, de réputation internationale – le Canadian Journal of Analytical Sciences and Spectroscopy (CJASS). Ce journal est depuis récemment disponible électroniquement à <http://www.cjass.ca>, et il est disponible à tous les membres de CSASS en étant inclus dans leur cotisation. Vos publications au CJASS peuvent maintenant être soumises en ligne!

Je voudrais remercier le docteur Holger Hintelmann, notre président de conférence, ainsi que son comité organisateur pour tout le travail accompli à la mise en marche de cette conférence. Il faut beaucoup de temps et d'effort pour en arriver à un si excellent programme technique. Je veux aussi remercier tous les exposants et commanditaires qui ont contribué à ICASS 2007. Sans leur généreux support, il ne serait pas possible de tenir conférence. Prenez s'il vous plaît le temps de visiter ces exposants pour exprimer votre appréciation personnelle.

Merci de participer à ICASS 2007, et j'espère que cette conférence vous plaira dans son aspect technique et aussi social.

Cordialement,
Teresa Switzer
Présidente CSASS



Why Should I Join the Canadian Society for Analytical Sciences and Spectroscopy?

The society was founded in Ottawa in the early 1950s and incorporated as a non-profit organization under the Canada Corporation Act on 9 January 1957 as the Canadian Association for Applied Spectroscopy. It was renamed and registered 31 May 1967 as The Spectroscopy Society of Canada. On 21 March 2005 the society was renamed and registered as the Canadian Society for Analytical Sciences and Spectroscopy.

Since those early days, the Society has expanded to include sections in the Province of Quebec, Ottawa, Toronto (Southern Ontario), Northern Ontario, Edmonton/Alberta, BC Interior, and Vancouver/Victoria. Throughout the year, programs of scientific and general interest are organized by the Local Sections for educational benefit of members and the public at large. The Society organizes an annual scientific conference, the International Conference on Analytical Sciences and Spectroscopy (ICASS). Workshops are usually offered in conjunction with ICASS.

CSASS has two major awards: the Gerhard Hertzberg Award and the Smiths Detection Spectroscopy Award for distinguished achievement in spectroscopy. There are also student travel awards given by CSASS for travel to ICASS, and MDS Sciex student

bursaries for students with high academic achievements and financial need. Local sections of CSASS support local science fair programs by providing judges and awards to students.

Since 1955, CSASS has published a journal, which has gone through several incarnations and is at present the internationally recognized Canadian Journal of Analytical Sciences and Spectroscopy. The journal is available electronically to members and is distributed to subscribing libraries both in Canada and abroad. A Newsletter is published three or four times a year and distributed to members.

CSASS cooperates with other scientific societies and organizations. For example, the CSASS and the Society for Applied Spectroscopy (USA) organize a tour speaker program. From time to time, other organizations collaborate with the CSASS at the ICASS meeting.

The annual membership fee supports CSASS activities, including awards and Local Section programs. Library subscriptions, corporate support, advertising, and a grant from CSASS support the cost of publishing the journal.

New membership received from October will remain valid until December of the following year

The Canadian Society for Analytical Sciences and Spectroscopy
P.O. Box 56018, Winnipeg, Manitoba, Canada, R3C 5R2

Regular Member: \$60 per year
Student Member: \$25 per year (free for 2007)

I would like to become a member of the CSASS and receive the Canadian Journal of Analytical Sciences and Spectroscopy and Canadian Spectroscopic News. Enclosed is my annual membership fee.

Name: _____ Tel: () _____

Fax: () _____

Email: _____

Fields of spectroscopic interest:



Pourquoi Joindre la Société Canadienne de Spectroscopie et des Sciences Analytiques?

La société a été fondée à Ottawa au début des années 50 et incorporée comme organisation à but non lucratif sous la loi canadienne des corporations le 9 Janvier 1957, sous le nom de Association Canadienne de Spectroscopie Appliquée. Elle fut rebaptisée et enregistrée le 31 Mai 1967 en Société de Spectroscopie du Canada. Le 21 Mars 2005, la société devint la Société Canadienne de Spectroscopie et des Sciences Analytiques.

Depuis ses débuts, la Société s'est étendue pour inclure des sections au Québec, à Ottawa, Toronto (Sud Ontario), au Nord de l'Ontario, à Edmonton/Alberta, en CB Intérieure, et à Vancouver/Victoria. Tout au long de l'année, des programmes d'intérêt scientifique et général sont organisés par les sections locales à des fins éducatives, pour les membres et le public en général. La Société organise une conférence scientifique, la Conférence Internationale en Sciences Analytiques et Spectroscopie (ICASS). Des ateliers sont habituellement offerts en conjonction avec ICASS.

CSASS offre deux prix importants : le Prix Gerhard Hertzberg Award et le Prix Spectroscopie Smiths Detection pour reconnaître des distinctions en spectroscopie. Il existe aussi des bourses de voyage pour les étudiants pour venir à ICASS, offertes par CSASS, et les bourses MDS Sciex aux

étudiants performants au niveau académique ou avec besoins financiers. Les sections locales de CSASS supportent les programmes locaux d'Expo Science en fournissant des juges et des prix aux étudiants.

Depuis 1955, CSASS publie un journal, qui est passé à travers plusieurs transformations pour être maintenant reconnu internationalement comme le Canadian Journal of Analytical Sciences and Spectroscopy. Le journal est disponible électroniquement pour les membres et il est distribué aux bibliothèques qui y souscrivent au Canada et à l'étranger. Un bulletin est aussi publié trois ou quatre fois l'an et distribué aux membres.

CSASS coopère avec d'autres sociétés et organisations savantes. Par exemple, CSASS et la Society for Applied Spectroscopy (USA) organisent un programme de circuit de conférenciers. De temps à autre, d'autres organisations collaborent avec CSASS à la conférence ICASS.

La souscription annuelle supporte les activités de CSASS, les prix et bourses offertes et les sections locales. Les abonnements de bibliothèques, le support corporatif, la publicité et une subvention de CSASS supportent les coûts de publication du journal.

Les nouvelles souscriptions reçues en Octobre seront valides jusqu'en Décembre de l'année suivante

Société Canadienne de Spectroscopie et des Sciences Analytiques
Boîte Postale 56018, Winnipeg, Manitoba, Canada, R3C 5R2

Membre régulier : \$60 par an
Membre étudiant: \$25 par an (gratuit en 2007)

Je voudrais devenir membre de CSASS et recevoir le Canadian Journal of Analytical Sciences and Spectroscopy et le bulletin Canadian Spectroscopic. J'inclus mon paiement annuel.

Nom: _____ Tél: ()

Télécopie: ()

Courriel: _____

Disciplines d'intérêts: _____



Notice of Meeting Avis de Convocation

The **Annual General Meeting** of the Canadian Society for Analytical Sciences and Spectroscopy will be on **June 26, 2007, during the ICASS meeting in Peterborough, Ontario during the lunch break**. All members in good standing with the Society are invited to attend. The agenda will include the Society's Finances, status of its journal, and the announcement of the new bylaws.

L'**Assemblée Générale Annuelle** de la Société canadienne des sciences analytiques et de spectroscopie se tiendra le **26 juin 2007, pendant le congrès ICASS à Peterborough, en Ontario pendant la pause du dîner**. Tous les membres en règle de la société sont invités à participer. L'ordre du jour inclura les états financiers de la société, la condition de son journal et l'annonce des nouveaux statuts.

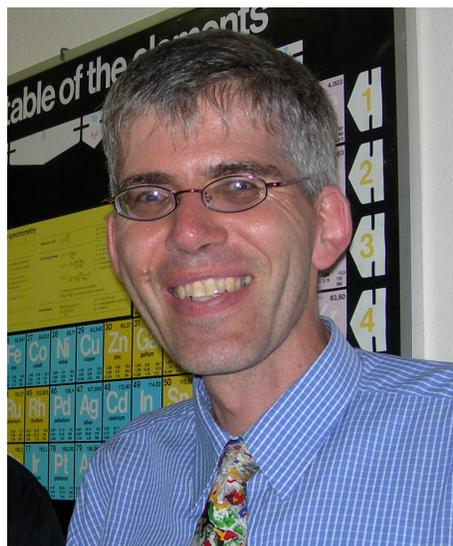
THE GERHARD HERZBERG AWARD

This award is given annually by the CSASS to a Canadian spectroscopist in recognition of outstanding achievement in the science of spectroscopy.

2007 Gerhard Herzberg Award Recipient:

Dr. Christian Reber

Christian Reber grew up in Switzerland, where he received his education in chemistry at the Universität Bern, specializing in inorganic chemistry. In 1989, he obtained his Ph.D. degree with a thesis on crystalline compounds of early first row d-block metals, work directed by Professor Hans U. Güdel. He then moved to North America to join Professor Jeffrey I. Zink's group at the University of California, Los Angeles for postdoctoral studies focused on excited electronic states of metal compounds probed by spectroscopic techniques. During this time, he also learned to apply theoretical models based on time-dependent quantum mechanics. Reber joined the faculty of the Université de Montréal in 1991 where he is currently a Professor of Chemistry, with an additional appointment since 2003 as Adjunct Professor at McGill University.



Research in the Reber group is aimed at the preparation, detailed exploration and understanding of the electronic structure of molecular solids. A unique combination of spectroscopic methods is used, consisting of steady-state and time-resolved luminescence, absorption and micro-Raman techniques, all at variable temperature and pressure. The spectroscopic results are relevant to many applications, ranging from new optical materials to chemical reactivity, making him and his team sought-after research collaborators.

Reber's previous honors include a CNC-IUPAC travel award (1997) and invited faculty fellowships at Université Louis Pasteur, Strasbourg (1998), Universität Bern (1999), Université Claude Bernard Lyon 1 (2004) and at UCLA (2007).

Past recipients:

1973	P. Krueger	1985	T.E. Gough	1997	I.S. Butler
1975	T.P. Schaefer	1986	I.C.P. Smith	1998	W.F. Reynolds and B.D. Sykes
1976	A. Cabana	1988	M.C.L. Gerry	1999	M. Pézolet
1977	C.L. Chakrabarti	1989	A.D. Bandrauk	2000	J.A. Weil
1978	H.L. Bernstein *	1990	J.L. Holmes	2001	A.R.W. McKellar
1979	R.N. Jones *	1991	G.M. Bancroft	2002	R. Sturgeon
1980	C. Sandorfy *	1992	B.R. Henry	2003	R.F. Aroca
1981	G.W. King	1993	M. Moskovits	2004	K.W.M. Siu
1982	J.C.D. Brand	1994	R.E. Wasylishen	2006	D. Bohme
1983	C.E. Brion	1995	P.T.T. Wong		
1984	H.H. Mantsch	1996	A.B.P. Lever		

* Deceased

THE SMITHS DETECTION AWARD

This award is sponsored by Smiths Detection. It is given to a Canadian spectroscopist in recognition of a significant contribution to the application of spectroscopy to analytical chemistry or to other technological problems relevant to industry, medicine, or the environment.

2007 Smiths Detection Award Recipient: **Dr. Yunjie Xu**

Yunjie Xu grew up on beautiful Lu Island in South East China. She received her B.Sc. in Chemistry and in Applied Mathematics from Xiamen University in 1988. She came to Canada in 1989 and earned a Ph.D. in molecular spectroscopy from the University of British Columbia in 1993. After working two years as a research associate at the National Research Council of Canada in Ottawa, she moved to the University of Alberta as a NSERC and a Killam postdoctoral fellow. She has been an assistant professor in the Chemistry Department there since 2003.



Dr. Xu's research focuses on spectroscopic detection and characterization of chirality and chiral recognition. Her group has designed and constructed several highly sensitive infrared detection systems for applications in molecular spectroscopy. Dr. Xu has published over 60 refereed research articles in leading scientific Journals including Science, Angew. Chem., J. Am. Chem. Soc., and Phys. Rev. Lett. She and her research group have delivery over 90 conference and invited presentations. She is a member of the Chemical Institute of Canada.

Past Recipients:

1977	G. Horlick	1993	T.B. McMahon
1978	H.L. Buijs	1994	J.D. McLaren
1979	I.C.P. Smith	1995	A. Lawrence and J.C. Scaiano
1980	J.L. Holmes	1996	D.C. Grégoire
1981	L.D. Hall	1997	B. Simard
1982	J.B. French	1998	J. Ripmeester
1983	R.M. Leblanc	1999	D. Burns
1984	A.J. Merer	2001	A. Stolow
1985	C.A. Fyfe	2002	M. Auger
1986	R.E. Sturgeon	2003	R. Guevremont
1988	D. Douglas	2004	M. Blades
1989	M.B. Comisarow	2005	H.P. Looock
1990	M. Falk	2006	V. Taguchi
1991	W. Doherty		
1992	C. Preston		

CONFERENCE SPONSORS

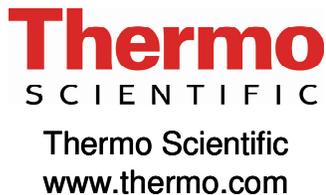
The ICASS 2007 exhibition will officially open Monday late afternoon and run through Tuesday until Wednesday afternoon. The exhibitor's hall will be located on the first floor of Gzowski College, Room 102.

Gold Sponsors



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www.varianinc.com

Exhibitors / Sponsors



Exhibitors – Cont'd



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www.scpscience.com



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www.ca.sgs.com



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www.tainstruments.com



Praxair
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Transition Technologies
www.transition.ca



Isomass
www.isomass.com



Canadian Society for Analytical
Sciences and Spectroscopy
www.csass.org



Canadian Thermal Analysis Society
www.ctas.org

CONFERENCE INFORMATION

Conference Organizing Committee

Conference Chair: Dr. Holger Hintelmann - hhintelmann@trentu.ca
Trent University, Chemistry Department
1600 West Bank Drive
Peterborough, Ontario, Canada – K9J 7B8
ph. 705 748-1011 x7659
fax. 705 748-1625

Organizing committee: Dr. David Ellis – davidellis@trentu.ca
Dr. Andrew Vreugdenhil – avreugdenhil@trentu.ca
Dr. Delphine Foucher – delphinefoucher@trentu.ca

CTAS Program Chair: Dr. Subhash Mojumdar - Subhash.Mojumdar@utoronto.ca
Centre for Bicomposites and Biomaterials Processing
Faculty of Forestry, University of Toronto
33 Willcocks Street
Toronto, Ontario, Canada – M5S 3B3

Exhibit Chair: Teresa Switzer - Teresa.Switzer@ontario.ca
Ontario Ministry of the Environment
125 Resources Road
Toronto, Ontario, Canada – M9P 3V6

Registration and Information Desk

All participants are requested to check in at the Registration Desk located on the first floor of Gzowski College in front of the Lecture Hall 114. We will be happy to provide any information needed.

Full Registrations include the conference program and book of abstracts; delegate pack; entry to all technical, plenary and poster events, and exhibition. The fee also includes the welcome reception; conference banquet; evening and afternoon socials; award ceremonies; 3 lunches; coffee, tea and refreshments during breaks.

Daily Registrations include the conference program and book of abstracts; delegate pack; admission to all scientific events, lunch, coffee breaks and social events of the specified day of registration.

Oral presentations – Speaker-Ready Room

Oral presentations are 20 minutes in length. Around five minutes of this time should be reserved for questions and comments from the audience. Each presentation room at the conference is set up with a conference computer, LCD projector, laser pointer and microphone. The conference computers (PCs) are set up with Microsoft Windows XP Professional and Microsoft PowerPoint

2003. Presenters should ensure that their presentations are compatible with this operating system and PowerPoint version.

Speakers are kindly asked to submit their presentation file to the conference secretariat or the Speaker Ready Room (1st floor of Gzowski College, Room 103) at least ½ day before your scheduled presentation. The Speaker Ready Room will be open from Sunday through Wednesday. There, you can also preview your presentation on the conference computer system and make minor adjustments as needed. For upload onto the central server, files will be accepted on CD-ROM, or on a flash drive or memory stick that plugs into a USB port.

Poster Presentations

Posters should not exceed 1 meter (36 inches) wide by 1.2 meters (48 inches) tall. Poster presenters are responsible for setup and take down their posters. The posters' numbers may be found in the scientific programme and the same numbers will be shown on the poster boards. Supplies (e.g. pins, tape) to display posters will be provided on site. Please, ask our organizers at the Registration Desk (1st floor of Gzowski College in front of the Lecture Hall 114).

Presenters will be asked to be on hand for discussion during the poster session (Monday Afternoon from 5.00 pm to 6.30 pm). Posters will stay on display during the whole conference.

PROGRAMME AT A GLANCE

	Jun-24 Sunday	Jun-25 Monday	Jun-26 Tuesday	Jun-27 Wednesday	Jun-28 Thursday
8:00					
9:00		Conference Opening Plenary Lecture	Parallel Sessions	Parallel Sessions	MC-Workshop Panel Discussion
10:00		Coffee Break	Coffee Break	Coffee Break	Coffee Break
11:00		Parallel Sessions	Parallel Sessions	Parallel Sessions	MC-Workshop Panel Discussion
12:00					
13:00		Lunch Break	Lunch Break	Lunch Break	Lunch Break
14:00		Parallel Session	LiftLock Cruise	Parallel Sessions	MC-Workshop Panel Discussion
15:00		Coffee Break		Coffee Break	Coffee Break
16:00	Registration Desk Open	Gerhard Herzberg Award		Parallel Sessions	MC-Workshop Panel Discussion
17:00		Opening of Exhibition	Smiths Detection Award	Conference Closing	
18:00		Poster Session			
19:00	Welcome Mixer	BBQ Dinner	Conference Banquet		
20:00					
21:00					

SOCIAL PROGRAMME

Sunday – June 24, 2007

18:00 - 21:00 **Welcome Mixer hosted by Thermo Scientific and Agilent Technologies**
Dining Hall (Cafeteria) – 2nd floor of Gzowski College

Monday – June 25, 2007

16:00 - 17:00 **The Gerhard Herzberg Award Ceremony**
Lecture Hall (114) – 1st floor of Gzowski College

18:30 - 21:00 **BBQ Dinner**
Gzowski College, outside in front of the Exhibitors Hall (Room 102)

Tuesday – June 26, 2007

13:30 - 16:00 **Sightseeing Cruise on the Trent-Severn Waterway**
All aboard! Cruise the Trent-Severn Waterway aboard the Island Princess III, rise to the top of the world famous *Peterborough Liftlock*, and explore the shores of the canal and its non stop scenery of beautiful homes/cottages and wildlife.

Boarding location: Little Lake Marina – 150 George Street

A bus transfer will be organized from Trent University to the Little Lake Marina (approximately 15 minutes). The meeting point will be at the bus stop outside in front of Gzowski College (2nd floor) at 13:30 p.m.

16:30 - 17:30 **The Smiths Detection Award Ceremony**
Lecture Hall (114) – 1st floor of Gzowski College

18:00 - 21:00 **Banquet Dinner**
The Great Hall – 1st floor of Champlain College

All social events are included in the fee for participants.

Please, note that extra tickets for the cruise and the banquet dinner for accompanying persons can be purchased at the registration desk at a cost of \$25.00 and \$50.00 per person, respectively. The price for the cruise includes also bus transport from Trent University to the boarding location.

SCIENTIFIC PROGRAMME – ICASS 2007

Monday – June 25, 2007 – Morning

Plenary Lecture

Lecture Hall 114

9:00 O01 Raymond March – *Ion Trapping in Quadrupole Fields; a Modern Saga*

COFFEE BREAK HOSTED BY CANADIAN LIFE SCIENCE

Environmental Applications of Mass Spectrometry

Room 117

Chair: David Ellis

10:30 O02 Vince Taguchi – *Are Halogenated Aminoxy Alcohols Disinfection By-Products in Treated Drinking Water? The Need for Accurate Masses in Chemical Ionization Experiments*

10:50 O03 Matthew Forbes – *Infrared Spectroscopy of Arginine Metal Cation Complexes: Direct Observation of Gas-phase Zwitterions*

11:10 O04 Janeen Auld – *Analysis of Hydroxyl Radical Initiated Photo-oxidation Products of beta-Pinene by Atmospheric Pressure Chemical Ionization Mass Spectrometry*

11:30 O05 Celine Gueguen – *Real Time Gas Measurements (CO₂, O₂, Ar) in Natural Waters Made by Membrane Inlet Mass Spectrometry*

11:50 O06 Chunyan Hao – *Matrix Effects in Liquid Chromatography Electrospray Tandem Mass Spectrometry Analysis of Emerging Organic Pollutants*

Monday – June 25, 2007 – Afternoon

Molecular Spectroscopy

Room 117

Chair: Subhash Mojumdar and Mazen Saleh

13:30 O07 Jonathan Morrison – *Long-Lived Rydberg States of NO*

13:50 O08 Nicholas Pieczonka – *The Photodynamics of Surface-Enhanced Resonance Raman Scattering*

14:10 O09 Darcy Burns – *Probing the Binding of BFRs to Thyroid Transport Proteins Using NMR Spectroscopy and Molecular Modeling*

14:30 O10 Heather Gamble – *Spectroscopic Monitoring of Perfluorocarbon Greenhouse Gases for Process Improvement in the Aluminium Industry*

14:50 O11 Douglas Goltz – *Spectroscopic Assessment of Historical Objects*

15:10 O12 Raymond March – *A Rationalization of Product Ion Mass Spectra of Monohydroxyflavones Using NMR combined with Chemical Computation*

The Gerhard Herzberg Award Lecture

Lecture Hall 114

16:00 O13 Christian Reber – *Colors and Light: Electronic States Probed by Spectroscopy*

Poster Session**Hallway**

- P01** Elize Ceschia – *Analysis of Polycyclic Aromatic Hydrocarbons (PAHs) Using an Atmospheric Pressure Chemical Ionization Triple Quadrupole Mass Spectrometer*
- P02** Delphine Foucher – *Variations in Mercury Stable Isotope Ratios in Low Level Environmental Samples*
- P03** Meher Chowdhury – *Novel Method for the Study of the Distribution of Metal and Metal-complexes in Aqueous Slurries of Sediments*
- P04** Mark Dzurko – *Mercury (Hg) Isotope Fractionation during Bioaccumulation in Aquatic Food Webs*
- P05** Chantal Blanchard – *The Application of DRC Technology to the Removal of Polyatomic Interferences during the Analysis of Precious Metals in Geological Samples by ICP-MS*
- P06** Oliver Burnham – *Mineralogical Controls on the Response of Geological Samples to Aqua Regia Leaching*
- P07** Andrei Izmer – *Application of Different Analytical Techniques for Determination of the Cesium Distribution in High Burnup Fuel Samples*
- P08** Don Parkinson – *Method Development for the Extraction of Volatiles from Molds by SPME-GC/MS*
- P09** Valbona Celo – *Trace Metal Content in Atmospheric PM_{2.5} Collected in Selected Canadian Locations: from Sampling to Analysis and Data Interpretation*
- P10** Jianjun Niu – *Bioaccessibility of Transition Metals in Airborne Particulate Matter*
- P11** Howard MacDonald – *Single-run ICP-MS Analysis of Major Cations, Phosphorous and Trace Metals and Heavy Metals in Natural and Waste Water Samples: QC/QA Protocol and Methodology Considerations*
- P12** Lizane Pamer – *Arsenic, Selenium and Indium as the Fingerprint of Smelter Contamination in Ombrotrophic Peats of the Sudbury, Ontario, Region*
- P13** Eavan O'Connor – *Determination of Selenium by HG-ICP-DRC-MS in the Brain Tissues of Laboratory-raised Mink Dosed with Selenium and Mercury*
- P14** Wang Zheng – *Mercury Isotope Fractionation during Volatilization of Hg(0) from Solution into the Gas Phase*
- P15** John Hechler – *What do Sequential Extractions Really Dissolve from Sediments – a XANES Study*
- P16** Pamela Koski – *Atmospheric Particulate Matter within the Sudbury Footprint*
- P17** Aimee Williamson – *Has the Signature Been Retained...the Chemistry of Lakes Downwind of a Smelter Region, Sudbury, Ontario*
- P18** Graeme Spiers – *Application of AFS to the Monitoring of Metals in Electronics Materials*
- P19** Darcy Burns – *An Accurate pKa Determination of Monomeric PFOA and its Environmental Implications*
- P20** Ralph Bona – *A Mass Balance of the Distribution of Bioavailable Hg²⁺ among Cellular Compartments of Genetically Modified E.Coli after Exposure to Hg Solutions*
- P21** Alexandre Rodrigue-Witchel – *Luminescence Spectra of Square-planar Pt(II) Complexes at Variable Pressure and Temperature*
- P22** Nader Kharouba – *The Processes of Nickel Partitioning in the Water Column of a Recovering Lake in the Sudbury, Ontario Region*

P23 Robert Hudson – *KINETEQL: A Sophisticated Excel Add-In Function for Computing Chemical Equilibria and Kinetics Using the Tableau Method*

Tuesday – June 26, 2007 – Morning

Environmental Applications of Atomic Spectroscopy

Room 117

Chair: Graeme Spiers

- 8:30 **O14** Joseph Caruso – *Metallomics Approaches to Answer Metabolomics Questions – the Synergy Between Elemental and Molecular MS*
- 8:50 **O15** Doreen Franke – *Mass-spectrometric Identification of Thioarsenates Explains Decrease of Arsenic Toxicity in Sulfidic Solutions*
- 9:10 **O16** Robert Hudson – *A Novel Method for Solid Phase Preconcentration of MeHg from Natural Water Samples via Thiourea-Catalyzed Ligand Exchange: Theory and Applications*
- 9:30 **O17** Sergei Boulyga – *Direct Isotope Analysis of Actinides and Particular Fission Fragments in Particles Using LA-MC-ICP-MS*
- 9:50 **O18** Wijdan Malik – *We are What We Breathe – An Examination of Potential Bioavailability of Metals in Aerosols*

COFFEE BREAK HOSTED BY AGILENT

Environmental Analysis

Room 117

Chair: Robert Hudson

- 10:40 **O19** Chris Metcalfe – *Challenges and Solutions for the Analysis of Pharmaceuticals and Personal Care Products in Environmental Samples*
- 11:00 **O20** Julie Bennett – *Composition of secondary Organic Particulate Matter from the Photo-oxidation of Hydrocarbons Using APCI/MS-MS*
- 11:20 **O21** Olivier Clarisse – *Methylmercury Speciation in a Stratified Lake Using New DGT Sensors*
- 11:40 **O22** Bob Helleur – *Thin Layer Chromatography Interfaced to Pyrolysis-GC/MS: Analysis of Crude Oils*

Tuesday – June 26, 2007 – Afternoon

The Smiths Detection Spectroscopy Award Lecture

Lecture Hall 114

- 16:30 **O23** Yunjie Xu – *Exploring Chirality and Chiral Recognition Using Spectroscopic and ab Initio Methods*

Wednesday – June 27, 2007 – Morning

Special Symposium: Where does ICP/MS stands?

Room 117

Chair: Teresa Switzer

- 8:30 **O24** Sam Houk – *The Scientific Contributions of ICP-MS*
9:10 **O25** Fergus Keenan – *Significant Milestones in the Development of ICP-MS: A Manufacturer's View of the Growth of ICP-MS from a Research Device to a Mature Instrument for Routine Analysis*
9:30 **O26** Kaveh Kahen – *ICP-Cell-MS; Norm or Exception?*
9:50 **O27** Doug Shrader – *The Collision Reaction Interface – A Simple Approach to Interference Management in ICP-MS*

COFFEE BREAK HOSTED BY DELTA SCIENTIFIC

Special Symposium: Where does ICP/MS stands?

Room 117

Chair: Teresa Switzer

- 10:40 **O28** Shulan Liu – *Effect of Pre-evaporation Tube on Arsenic Speciation Analysis*
11:00 **O29** Michael Minnich – *Clinical ICP-MS for Biomonitoring and Chemical Terrorism Preparedness*
11:20 **O30** Joseph Caruso – *Screening Organophosphorus Nerve Agent Degradation Products by ³¹P ICP-MS*
11:40 **O31** Scott Tanner – *New Reagents and Instrument for Multiplexed Single Particle BioAssay with ICP-MS*

Wednesday – June 27, 2007 – Afternoon

Special Symposium: Where does ICP/MS stands?

Room 117

Chair: Teresa Switzer

- 13:30 **O32** Kym Jarvis – *Has ICP-MS Delivered All It Promised?*
13:50 **O33** Chuck Douthitt – *Where ICP-MS Stands? A Manufacturer's Point of View*
14:10 **O34** Don Chipley – *ICP-MS – The Users Point of View*
14:30 **O35** Diane Beauchemin – *A Long-time User's Point of View on Where ICP-MS stands*

Special Symposium: Where does ICP/MS stands?

Room 117

Chair: Teresa Switzer

- 15:10 **O36** Fred Smith – *ICP-MS: As You Like It*
15:30 **O37** Ramon Barnes – *Modeling the Inductively Coupled Plasma: A Historical Review of Computer Simulations from Emission to Mass Spectrometry*
15:50 **O38** Graeme Spiers – *The ICP-MS Goes Environmental – Adventures with a New Toy*

SCIENTIFIC PROGRAMME – CTAS 2007

Monday – June 25, 2007 – Morning

Plenary Lecture

Lecture Hall 114

9:00 O01 Raymond March – *Ion Trapping in Quadrupole Fields; a Modern Saga*

COFFEE BREAK HOSTED BY CANADIAN LIFE SCIENCE

Training Session

Room 115

10:30 O39 Charles Potter (TA Instruments) – *Industrial Applications of Calorimetry and Thermal Analysis*

11:30 O40 Frank Palmisano (Mettler-Toledo Inc.) – *DSC-Microscopy: Seeing is Believing*

Monday – June 25, 2007 – Afternoon

Training Session

Room 115

13:30 O41 Elisabeth Kapsch (Netzsch Instruments Inc.) – *Thermal Analysis Coupled to Online Evolved Gas Analysis*

Vendor Presentations

Room 115

14:30 Netzsch Instruments Inc.

14:45 Mettler-Toledo Inc.

15:00 TA Instruments

The Gerhard Herzberg Award Lecture

Lecture Hall 114

16:00 O13 Christian Reber – *Colors and Light: Electronic States Probed by Spectroscopy*

Poster Session

Hallway

P24 G. Madhurambal – *DSC, TGA, DTA, SEM and FT-IR Spectral Studies, and Influence of 1, 10-phenanthroline on Potassium Hydrogen Phthalate Crystals*

P25 Mazen Saleh – *Thermoanalytical Characterization and Antibacterial, Antiyeast and Antifungal Activities of Mg(II) and Cu(II) Compounds with Bioactive Ligands*

P26 G. Madhurambal – *Characterization of ADP and KDP Crystals Using TGA-DTA, FTIR, XRD, SEM and Microhardness*

P27 Mazen Saleh – *Thermal, Spectral and X-Ray Analysis and Fungicidal Activities of Novel Fungicides*

Tuesday – June 26, 2007 – Morning

Plenary Lecture

Room 115

8:30 **O42** Pearl Lee-Sullivan – *The Matrix: Evolutions, Gaining Insight from Thermal Analysis*

Open Forum

Room 115

9:10 Moderator: Pearl Lee-Sullivan

Technical Session

Room 115

9:30 **O43** Jacky Tang – *Cooling Rate Studies of a Polycarbonate/Acrylonitrile-Butadiene-Styrene Polymer Blend by DSC*

9:45 **O44** Feng Tian – *Absolute Measurements of Thermal Conductivity of Acrylic Acid Solution by the Transient Hot Wire Technique*

10:00 **O45** Roshan Shetty – *Raman Spectroscopy Resolution Limits Overcome by Sub-100nm Thermal Analysis*

COFFEE BREAK HOSTED BY AGILENT

Technical Session

Room 115

10:40 **O46** Frank Palmisano – *DSC with the TGA/SDTA851e Taking Weight Loss into Account*

10:55 **O47** Soubir Basak – *Thermal Decomposition of Iron Compounds Modified by Hydrazine*

11:10 **O48** Subhash Mojumdar – *Thermoanalytical Properties of Wheat Gluten Protein Films*

11:25 **O49** Daniel Martineau – *Kinetics of the Thermal Decomposition of Nitrocellulose*

11:40 **CTAS Annual General Meeting**

Tuesday – June 26, 2007 – Afternoon

The Smiths Detection Spectroscopy Award Lecture

Lecture Hall 114

16:30 **O23** Yunjie Xu – *Exploring Chirality and Chiral Recognition Using Spectroscopic and ab Initio Methods*

Wednesday – June 27, 2007 – Morning

Technical Session

Room 115

- 8:30 **O50** Tulika Mojumdar – *Characterization of Polymeric Materials Using Laser-induced Breakdown Spectroscopy (LIBS) and TGA, DTG and DSC*
- 8:45 **O51** Koyar Rane – *Hydrazine Method of Synthesis of Al₂O₃: Thermal Decomposition of Aluminum Carboxylates*
- 9:00 **O52** G. Madhurambal – *Growth and Characterization of 2-bromo-4-chloroacetophenone (BCAP) Crystals*
- 9:15 **O53** Mazen Saleh – *The Use of Insoluble Potato Fiber as a Microbial Carrier for Bioremediation*
- 9:30 **O54** Subhash Mojumdar – *Synthesis of Nanosize Nickel Ferrite at Relatively Lower Temperature Using Novel Precursor Combustion Technique*
- 9:45 **O55** Koyar Rane – *Hydrazine Method of Synthesis of Al₂O₃: Thermal Decomposition of Aluminum Hydroxides*
- 10:00 **O56** G. Madhurambal – *TGA, DTA and UV, FTIR and NMR Spectral Characterization of Benzophenone and Mixed Crystal of BP and 2, 4 Dinitro Phenyl Hydrazone of Benzophenone*

COFFEE BREAK HOSTED BY DELTA SCIENTIFIC

Technical Session

Room 115

- 10:45 **O57** Tulika Mojumdar – *FTIR Spectroscopy and Thermal Analysis in Characterizing Various Materials*
- 11:00 **O58** Subhash Mojumdar – *Special Cement Blend Bound in Geosynthetics Liner: Application in Mechanical and Anti-rust Protection of Pipelines*
- 11:15 **O59** Koyar Rane – *Oxygen Scavengers in Boiler Feed Water: Thermal Studies of Cobalt(II) 3,4 Diaminotoluene and Co(II) Diaminotoluene Hydrazinate Complexes*
- 11:30 **O60** G. Madhurambal – *Effect of Low and High Concentrations of KCl Dopant on ADP Crystals*
- 11:45 **O61** Tulika Mojumdar – *The Applications of Raman Spectroscopy and Thermal Analysis Characterization of Various Materials*

Wednesday – June 27, 2007 – Afternoon

Technical Session

Room 115

- 13:30 **O62** Subhash Mojumdar – *Synthesis, Characterization, Fungicidal and Bactericidal Activities of Metal Diethyldithiocarbamate Fungicides*
- 13:45 **O63** G. Madhurambal – *Solution Grown Benzophenone: Study of the Thermal Properties, Nucleation Parameters, Induction Period and Interfacial Energy*
- 14:00 **O64** Ranjit Verma – *Thermal Analysis of 2-oxocyclopentanedithiocarboxylato Complexes of Iron(III), Copper(III) and Zinc (II) Containing Pyridine or Morpholine as the Second Ligand*

SCIENTIFIC PROGRAMME – MC WORKSHOP

Thursday – June 28, 2007 – Morning

Plenary Lecture

Room 115

8:30 – 9:00 Chuck Douthitt – *The Development and Dissemination of MC-ICPMS Technology, with an Overview of Current Applications*

9:00 – 10:00 Introduction of Research Groups

COFFEE BREAK

Panel Discussion: Mass Bias – Mass Fractionation

Room 115

10:30 – 10:45 Anthony Nonell – *Application of MC-ICP-MS to Nuclear Problematics*

10:45 – 11:00 Togwell Jackson – *Mass-independent Variation in the Stable Isotope Composition of Mercury in Methylmercury Accumulated by Freshwater Food Web Organisms*

11:00 – 11:15 Don Chipley – *MC-ICP-MS, The Nightmare of Matrix, Mass Bias and Mass Fractionation*

11:15 – 12:00 Open Discussion

Thursday – June 28, 2007 – Afternoon

Plenary Lecture

Room 115

13:30 – 14:00 Peter Stow – *MC-ICP-MS faults, cures and other fishy tales*

Panel Discussion: Transient Signal – Speciation

Room 115

14:00 – 14:15 Mark Dzurko – *Determination of Isotope Ratios from Transient Signals evolved from MC-ICP-MS Measurements*

14:15 – 15:00 Open Discussion

COFFEE BREAK

Panel Discussion: Matrix Effect – Sample Preparation

Room 115

15:30 – 15:45 Nagmeddin Elwaer – *Selective Separation of Selenium (IV) by Cellulose Thioglycollic Acid Powder*

15:45 – 16:00 Karima Benkhedda – *Fe Isotopic Analysis by MC-ICP-MS in Nutritional Studies: Beyond the Challenges*

16:00 – 16:15 Qianli Xie – *Potential Interferences in MC-ICP-MS and Impacts on High Precision Isotope Measurements: Using B as an Example*

16:15 – 17:00 Open Discussion

ABSTRACTS – ORAL PRESENTATIONS

001 Ion Trapping in Quadrupole Fields; a Modern Saga

Raymond March

The quadrupole ion trap, QIT, was surely the most atypical mass spectrometer to be introduced in the twentieth century. In a world of large sector instruments, the QIT was small; ion paths within the QIT were torturous rather than linear; ion/neutral collisions were said to be desirable rather than an anathema; and the pressure within the QIT was some three orders of magnitude higher than in a sector instrument. Yet the QIT is now placed securely within the arsenal of sophisticated analytical instruments of high versatility and sensitivity. The pace of instrument development of the QIT has been meteoric and the degree of acceptance of this instrument has been extraordinarily high. It is estimated that some 6,500 QIT instruments have been purchased at an average cost of \$100,000; thus, some $\$6.5 \times 10^8$, a substantial fraction of the funds allocated to the purchase of mass spectrometers, has been directed to the purchase of QIT instruments. A largely personal view of the history and development of the quadrupole ion trap during the past 30 years will be presented, together with a review of recent developments that include the highly-charged ion trap (HCT), the linear ion trap (LIT), the mini-cylindrical ion trap (mini-CIT), arrays of mini-CITs, the digital ion trap (DIT), and the rectangular ion trap (RIT).

002 Are Halogenated Aminoxy Alcohols Disinfection By-products in Treated Drinking Water? The Need for Accurate Masses in Chemical Ionization Experiments

Vince Taguchi, Moschoula Trikoupi, Jie Xing, Karl Jobst, Johan Terlouw

At the Ministry of the Environment (MOE), there have been on-going efforts to identify selected unknown disinfection by-product (DBPs) in extracts from treated drinking water. In 2001, two new DBPs were tentatively identified as 1-aminoxy-1-chlorobutan-2-ol (DBP-A) and 1-aminoxy-1-bromobutan-2-ol (DBP-B) respectively. In 2002, the NIST02 database became available. It contains the EI mass spectra of 4-chloro-2-methylbutan-2-ol and 3-bromo-2-methylbutan-2-ol whose fragment ion patterns are close to those of DBP-A and DBP-B respectively. This prompted us to reexamine the presence of the aminoxy moiety in the original structure proposals. The EI mass spectrum of DBP-A is very close to the NIST02 spectrum of 4-chloro-2-methylbutan-2-ol. The CI data are consistent with DBP-A having the elemental composition $C_5H_{11}ClO$ ($M=122$). The weak ions in the high mass region, at m/z 140 and m/z 142, represent the chlorine isotopes of its ammonium adduct $[M+NH_4]^+$ rather than the protonated form of the previously proposed "aminoxy" structure. However, the retention time of an authentic sample of 4-chloro-2-methylbutan-2-ol did not match that of DBP-A. The only other $C_5H_{11}ClO$ isomer expected to show similar EI dissociation characteristics is 3-chloro-2-methylbutan-2-ol. An authentic sample of this isomer was prepared to confirm the structure of DBP-A. The EI mass spectrum of DBP-B is very close to the NIST02 spectrum of 3-bromo-2-methylbutan-2-ol. The CI mass spectrum is consistent with DBP-B having the elemental composition $C_5H_{11}ClO$ ($M=166$). The structure of DBP-B was confirmed through the analysis of an authentic sample of 3-bromo-2-methylbutan-2-ol.

003 Infrared Spectroscopy of Arginine Metal Cation Complexes: Direct Observation of Gas-phase Zwitterions

Matthew Forbes, Matthew Bush, Nick Polfer, Jos Oomens, Robert Dunbar, Evan Williams, Rebecca Jockusch

The structure of cationized arginine complexes $[Arg+M]^+$, ($M^+=H^+, Li^+, Na^+, K^+, Rb^+, Cs^+$ and Ag^+) and protonated arginine methyl ester $[ArgOMe+H]^+$ have been investigated in the gas phase using calculations and infrared action spectroscopy in the region $800-1900\text{ cm}^{-1}$. Infrared multi-photon dissociation (IRMPD) has been carried out using the tuneable free-electron laser for ion excitation (FELIX) in conjunction with Fourier transform ion cyclotron resonance mass spectrometry (FTICR-MS). The structure of arginine in these complexes depends on the identity of the cation, adopting either a zwitterionic (salt-bridge) or non-zwitterionic (charge-solvated) conformation. As ArgOMe cannot form a zwitterion, it provides a signature

infrared fingerprint for the non-zwitterion conformation, exhibiting a band above 1700 cm^{-1} assigned to the carbonyl stretch. This diagnostic band is observed for $[\text{Arg}+\text{M}]^+$, ($\text{M}^+=\text{H}^+, \text{Li}^+, \text{Ag}^+$) clearly indicating that these complexes are also non-zwitterionic. In contrast, for K^+ , Rb^+ and Cs^+ the measured IR-action spectra show that in these complexes, arginine is a zwitterion. $[\text{Arg}+\text{Na}]^+$ exists predominantly as a zwitterion; however, a small contribution from a charge-solvated conformer is also observed. Thus, for the alkali metal complexes there is a clear trend between metal ion size and zwitterion stability. However, the Ag^+ complex adopts a charge-solvated conformation in the gas phase, deviating from this trend. The conformational landscape of the Arg-cation complexes has been investigated using electronic structure theory calculations. Experiment and theory show good agreement; the computed spectra of the global minimum-energy conformers provide the best match to the measured spectra.

O04 Analysis of Hydroxyl Radical Initiated Photo-oxidation Products of beta-Pinene by Atmospheric Pressure Chemical Ionization Mass Spectrometry

Janeen Auld, Julie Bennett, Don Hastie

A multitude of hydrocarbons arise in the atmosphere from both anthropogenic and biogenic sources. These hydrocarbons can undergo hydroxyl radical initiated photo-oxidation resulting in a complex system of organic products, which impact both climate, visibility, and human health. The formation mechanisms for these products have been proposed however remain unconfirmed. Using the York University Smog Chamber the hydroxyl radical initiated oxidation mechanism of beta-pinene is being investigated. Oxidation products have been identified and monitored using an atmospheric pressure chemical ionization triple quadrupole mass spectrometer. Identification has been accomplished using Q1MS scans to survey the contents of the chamber during the reaction. Subsequently, tandem mass spectrometry or MSMS has been used to acquire the fragmentation patterns of suspected products, which are used to elucidate the structure. Time profiles of identified products have been acquired using multiple reaction monitoring (MRM) scans where a unique precursor and product ion pair are monitored simultaneously over the course of an experiment. From these time profiles valuable mechanistic information has been obtained. To further this information experiments with varying NO_x levels have been carried out in order to examine and understand the available pathways of oxidation.

O05 Real Time Gas Measurements (CO_2 , O_2 , Ar) in Natural Waters Made by Membrane Inlet Mass Spectrometry

Céline Gueguen

Dissolved gases in surface waters play an important role in global climate regulation and serve as valuable tracers of biological, chemical and physical processes. Simultaneous measurements of inert (Ar) and biologically active gases (O_2 , CO_2) have been used to investigate photosynthesis/respiration in the natural waters using membrane inlet mass spectrometry (MIMS). The calibration of pCO_2 measurements by MIMS is reported for the first time using two independent methods of temperature correction. Multiple calibrations showed that the MIMS method provides pCO_2 measurements that are consistent with those obtained by standard techniques, with accuracy better than $0.8\ \mu\text{atm}$. The O_2/Ar ratio measurements were calibrated with air-equilibrated seawater standards stored at constant temperature ($0 \pm 1^\circ\text{C}$). The reproducibility of the O_2/Ar standards was better than 0.07%. Application of MIMS to the Southern Ocean has revealed significant small-scale heterogeneity in the distribution of pCO_2 and biologically induced O_2 supersaturation (DO_2/Ar) undetectable using traditional methods. The influence of thermal fronts and biological activities on CO_2 and O_2 concentrations will be discussed.

O06 Matrix Effects in Liquid Chromatography Electrospray Tandem Mass Spectrometry Analysis of Emerging Organic Pollutants

Chunyan Hao, Xiaoming Zhao and Paul Yang

The study on emerging organic pollutants (EOPs) in the environment has drawn more and more attention since last decade. Liquid chromatography with electrospray tandem mass spectrometry (LC/ESI-MS-MS) technique is demonstrated to be a powerful tool for the determination of these EOPs. However, due to the complex nature of environmental samples, matrix effects are a common issue in the analysis that is

impossible to completely eliminate. In this study, using an Applied Biosystems/MDS Sciex 4000Qtrap mass spectrometer coupled with an Agilent 1100 liquid chromatograph with electrospray ionization interface, we explored matrix effects during LC/ESI-MS-MS analysis of EOPs in detail and demonstrated the best approach to compensate for these effects. Our experimental results showed matrix effects existed in the form of signal (electrospray ionization efficiency) suppression or enhancement, and the level of suppression or enhancement of certain EOPs was affected by sample type, volume, pH, sample extract storage time, and the ionization mode employed. Also demonstrated was the use of isotope-labelled analogues provided the best tool to offset matrix effect for native EOPs. With more and more isotope-labelled analogues available, the new labor and time-saving strategy is to use isotope-labelled surrogates to correct for matrix effects and obtain accurate, high-quality analytical data.

007 Long-Lived Rydberg States of NO

Jonathan Morrison

Reported lifetimes of 1.2 μs for $n \geq 200$ p-orbitals first observed by Reiser *et al* ^[1], deviated from the anticipated value by at least two orders of magnitude for isolated NO molecules. Chupka proposed a mechanism for these long-lived Rydberg states based on Stark mixing of orbital angular momentum states ^[2]. This l-type mixing creates what is referred to as a 'magic region' observed in zero kinetic electron spectroscopy (ZEKE) experiments. This 'magic region' consists of energy levels with lifetimes that far exceed theoretical predictions. We have observed resolved spectra of $\sim 6.25 \mu\text{s}$ signal that can be dually assigned to p - and f -series for the upper threshold of ionic $N^+ = 0$ and 2, respectively ^[3]. Spectra show distinct lines down to $n \geq 30$ level that can not be attributed to field ionization which is characterized by change in ionization threshold of $E = 1/2(eF/\hbar)^{1/2} \approx 6 \text{ cm}^{-1}(F \text{ cm/V})^{1/2}$. It is believed collective effects dominate the lifetime extension of these states. These collective effects believed to be instigated by molecular Rydberg-Rydberg collisions, having strong dependence on Rydberg-density. We employed several different methods to alter Rydberg density and observed a systematic change in signal at a critical value. Temperature dependence was also investigated and observed to have an effect. Our molecular source consists of a skimmed, free-jet expanded NO beam seeded in helium. We estimate a cold rotational temperature of approximately 5-10 K based on REMPI spectra.

[1] Reiser, G., Habenicht, W., Muller-Dethlefs, K., Schalg, E.W. *Chem. Phys. Lett.* **152**. 119.

[2] Chupka, W.A. *J. Chem. Phys.* **98**. 4520.

[3] Vrakking, M.J.J., Lee, Y.T. *Phys. Rev. A.* **51**(2).

008 The Photodynamics of Surface-Enhanced Resonance Raman Scattering

Nicholas Pieczonka, Ricardo Aroca

Surface-enhanced resonance Raman scattering (SERRS) is a double resonance phenomenon where the exciting photon matches both the molecular electronic excitation and the plasmon resonance of a metallic nanoparticle or a surface protrusion. For many years, experimentalists have realized that the SERRS signal rapidly decays with time. The photodynamics of isolated dye molecules and that of dyes and non-absorbing molecules on metal surfaces have been studied both theoretically and experimentally. However, a detail discussion of the SERRS signal decay is not available. Here, we have looked at the signal decay of the SERRS of several systems. An attempt is made to discuss the many factors that impact the measured SERRS signal, including the role of competition between the excitation rate, the deactivation rate, and the rate of photobleaching. As well, we will explore how information derived from such photodynamical studies, could give additional insight on the phenomena of SERRS itself.

009 Probing the Binding of BFRs to Thyroid Transport Proteins using NMR Spectroscopy and Molecular Modeling

Darcy Burns, Gord Balch, Mehran Alaei, Chris Metcalfe

There is evidence that brominated flame retardants (BFRs) may disrupt the thyroid endocrine system of vertebrates by competitively inhibiting thyroid hormone binding to transport proteins such as human transthyretin (hTTR). For instance, *in vitro* studies found that an unidentified metabolite of BDE47, generated by CYP2B-enriched liver microsomes, was capable of competitively inhibiting >60% of

thyroxine (T4) from binding to human transthyretin (hTTR). NMR spectroscopy combined with molecular modeling comprise a unique approach for investigating protein-ligand interactions and thus are ideally suited to probe the capacity of BFRs to bind thyroid hormone transport proteins. We have applied 1D ¹H saturation transfer difference (STD) NMR spectroscopy to quantitatively evaluate binding between bisphenol A (BPA) and hTTR as well as to measure the relative inhibition potencies of L-thyroxine (T4), selected BFRs and BFR metabolites. Automated docking was performed to help determine the detailed structural nature of BFR binding by hTTR. We have found that these techniques can be used as a general tool to study the action of emerging contaminants, specifically BFRs and their metabolites, on thyroid regulation in vertebrate species.

O10 Spectroscopic Monitoring of Perfluorocarbon Greenhouse Gases for Process Improvement in the Aluminium Industry

Heather Gamble, Gervase Mackay

The potent greenhouse gases tetrafluoromethane (CF₄) and hexafluoroethane (C₂F₆) are present in emissions from various industrial processes including the primary smelting of aluminium. Over the past decade and more government and industry have worked together both to reduce total emissions, and to obtain data with the goal of obtaining an accurate global inventory of the quantities of these gases present in the atmosphere. Recommended best practices involve continuous, *in situ*, real time measurement of perfluorocarbon levels in industrial exhaust ducts. Various techniques have been used, including mass spectrometry, mid-IR tunable diode laser spectroscopy, and FTIR spectroscopy. The above techniques all give satisfactory data, and measurements using these techniques have been used to improve process efficiency and reduce emissions. The best technique is one which is simple and inexpensive to apply, thus encouraging ongoing rather than periodic monitoring. FTIR spectrometers can satisfy this requirement. Ongoing advances in instrument technology are making prospects for ongoing measurement and process optimisation ever brighter.

O11 Spectroscopic Assessment of Historical Objects

Douglas Goltz, Kimberly Charleton, Edward Cloutis, Mike Attas

Numerous spectroscopic approaches that have been developed by scientists have been adapted by conservators and conservation scientists for studying cultural objects. This presentation will describe the feasibility of using a dry cotton bud to lightly contact a painted surface for removing a small quantity of pigment (<1 µg). This sampling approach causes no visible damage to a painted surface. Pigments were extracted with concentrated HNO₃ prior to analysis with graphite furnace AAS and ICP-MS. Identifying pigment metals in combination with Raman spectroscopy can allow identification of individual and mixed pigments. Visible and near IR hyperspectral imaging are powerful spectroscopic tools for the examination of historically important documents. Imaging in the wavelength range of 420 to 1100 nm was ideal for a number of applications including the enhancement of faint text or distinguishing overlapping text. Hyperspectral imaging can also be adapted for mapping stains on parchments as well as for assessing the spatial distribution of inks that were fugitive.

O12 A Rationalization of Product Ion Mass Spectra of Monohydroxyflavones using NMR Combined with Chemical Computation

Raymond March, Darcy Burns, David Ellis, Errol Lewars, Hongxia Li

A method is presented for the estimation of ¹³C chemical shifts for carbon atoms in protonated and deprotonated flavonoids molecules; in principle, this method can be applied to ions in general. Product ion formation from protonated and deprotonated molecules of flavone and 3-, 5-, 6-, 7-, 2'-, 3'-, and 4'-hydroxyflavones is due to either cross-ring cleavage of the C-ring (retro-Diels-Alder reaction) or to cleavage of a C-ring bond followed by loss of either a small neutral molecule or a radical. The total product ion abundance ratio of C-ring cross cleavage to C-ring bond cleavage, Y, varies by a factor of 660 for deprotonated monohydroxyflavones, that is, from 0.014:1 to 9.27:1. The magnitude of Y, which is dependent upon the relative bond orders within the C-ring of the protonated and deprotonated molecules of monohydroxyflavones, can be rationalized on the basis of the magnitudes of the pseudo-¹³C chemical

shifts. Because experimental ^{13}C chemical shifts determined by nuclear magnetic resonance spectroscopy vary linearly with atomic charges computed using the PM3 method, pseudo- ^{13}C chemical shifts for atoms in protonated and deprotonated molecules can be estimated from computed atomic charges for such atoms using the above linear relationship.

O13 Colors and Light: Electronic States Probed by Spectroscopy

Christian Reber

Electronic spectroscopic experiments on transition metal compounds continue to play a key role in the development of inorganic and organometallic chemistry. These compounds are also of interest as important building blocks for new functional materials and in molecular and optical technology. Detailed luminescence, absorption and (resonance) Raman spectroscopic experiments ⁽¹⁾ can be used to characterize their electronic structure, simultaneously these experiments also reveal many interesting materials properties. Illustrative experimental results will be presented and analyzed with quantitative theoretical models ⁽²⁾.

1. Reber, C.; Grey, J. K.; Lanthier, E.; Frantzen, K. A., *Comments on Inorg. Chem.* 2005, 26, 233.

2. Gonzalez, E.; Rodrigue-Witchel, A.; Reber, C., *Coord. Chem. Rev.* 2007, 251, 351.

O14 Metallomics Approaches to Answer Metabolomics Questions – the Synergy Between Elemental and Molecular MS

Joseph Caruso

Metals and metal-containing compounds are known to play important roles in many biological processes. Plant studies involve better unraveling of the metabolic processes in wild type and genetically enriched plants, as such studies can provide fundamental information on generating a better phytoremediating plant. Another recent study involves cerebrospinal fluid (CSF) from stroke patients with and without the further complication of vasospasm – a seriously life threatening condition. Our first studies in this area are to compare phosphopeptides from low abundance and lower M.W. proteins. This talk will describe the progress in these areas using chromatographically coupled mass spectrometric methods. For plants, the approach involved the overexpression of a gene isolated from the Se hyperaccumulator, *A. bisulcatus*, which encodes for selenocysteine methyltransferase (SMT) to methylate SeCys to form Se-(methyl)-selenocysteine (MeSeCys), a non-proteinogenic amino acid, thus diverting the Se flow away from SeCys and subsequent production of SeMet, both of which can be mis-incorporated into proteins, altering their native structure and function. Decreasing SeCys levels represent an important Se tolerance strategy. The studies with CSF made important use of detecting ^{31}P at its only natural isotope by ICPMS as a means of screening for P containing peptides. Studies were done both with std. LC-ICPMS and with a newly designed capillary LC-ICPMS interface.

O15 Mass-spectrometric Identification of Thioarsenates Explains Decrease of Arsenic Toxicity in Sulfidic Solutions

Doreen Franke, Dirk Wallschlaeger, Britta Planer-Friedrich

Upon addition of increasing concentrations of sulfide (0.01 mg/L to 1000 mg/L) to solutions containing 100 mg/L arsenite bioluminescence of the marine bacteria *Vibrio fischeri* decreased. Minimum inhibition of bioluminescence (30 %) was determined at 100 mg/L sulfide, compared to 90 % in the absence of sulfide. In previous research, formation of less toxic thioarsenic species was proposed to be the reason for the observed decrease in toxicity, but no species identification was performed. We did arsenic speciation using anion-exchange chromatography with an alkaline eluent (20-100 mM NaOH). Simultaneous ICP-MS on-line detection of arsenic (as AsO^+ , $m/z = 91$) and sulfur (as SO^+ , $m/z = 48$) used the dynamic reaction cell technology with O_2 as reaction gas. Retention time match with synthetic standards, for which molecular electrospray mass-spectra have been obtained before, confirms the identification of the observed arsenic species as mono-, di-, and trithioarsenate. Experiments with commercial arsenite and arsenate standards and previously synthesized mono- and trithioarsenate standards show a decreasing toxicity from arsenate via arsenite to trithioarsenate and monothioarsenate. The latter one exhibited the lowest toxicity potential. These results contradict previous assumptions of decreasing toxicity with an

increasing number of SH-groups, but confirm the general trend that formation of thioarsenic species decreases arsenic toxicity potential in the environment. This result is important since recent field studies within our work group have shown that thioarsenic species predominate arsenic speciation in sulfidic near-neutral to alkaline waters, such as Yellowstone's geothermal hot springs or the anoxic bottom waters of Mono Lake.

O16 A Novel Method for Solid Phase Preconcentration of MeHg from Natural Water Samples via Thiourea-Catalyzed Ligand Exchange: Theory and Applications

Robert Hudson, Brian Vermillion

Ultratrace analysis of dissolved MeHg in freshwater samples requires both dissociation of MeHg from strong ligands in the sample matrix and preconcentration prior to chromatographic analysis. Existing solid phase extraction methods generally do not concentrate MeHg effectively from natural water samples containing high levels of dissolved organic matter. The addition of 10-60 mM thiourea quantitatively releases MeHg from the dissolved matrix of freshwater samples by forming MeHgTU⁺, a species that quantitatively exchanges with thiol-functionalized resins during column loading. The off-line columns can be eluted with acidic thiourea and the MeHg analyzed by Hg-thiourea complex ion chromatography with CVAFS detection. In a field study of the Grand Calumet watershed (Indiana, USA), routinely >90% matrix spike recoveries were observed with good precision in samples of water from wetland pools and sediment porewaters. The method detection limit is 0.29 pg absolute or 0.007 ng/L in 40 mL samples. Based on our knowledge of the chemistry of the process, breakthrough volumes should depend on [TU] and [H⁺]. Formation of artifactual MeHg is minimal. The potential range of applications of the pre-concentration method – sample types and methods of MeHg detection – will be considered.

O17 Direct Isotope Analysis of Actinides and Particular Fission Fragments in Particles Using LA-MC-ICP-MS

Sergei Boulyga, Thomas Prohaska

Uranium and plutonium isotopic ratio analysis in micrometer-sized particles is of greatest interest for nuclear forensics. The isotopic information indicates possible use in reactor fuel or nuclear explosives and can reveal undeclared use of nuclear materials. At present several methods are employed for uranium and plutonium analysis in radioactive single particles including nuclear track radiography, TIMS, SIMS or SEM^[1]. The present work describes the development of a rapid and ultrasensitive analytical procedure based on nuclear track radiography and subsequent laser ablation inductively coupled plasma mass spectrometry with multiple ion counters (LA-MC-ICP-MS) for direct analysis of both actinides (U and Pu isotopes) and particular fission products (Ru and Nd isotopes) in environmental microsamples. Solid sampling by laser ablation ICP-MS allows direct and rapid analysis of microsamples and achieving high sensitivity for long-lived radionuclides in micrometer-sized particles. Thus, uranium isotope ratios were measured in single particles of diameters of about 1 micrometer. The zoom lens for ion focusing in MC-ICP-MS was found advantageous for a rapid switching between actinide isotopes and fission product isotopes when determining both actinides and fission products in the same particle. The developed method was applied for investigation of isotopic ratios of corresponding elements in 'hot' particles originating from the Chernobyl vicinity.

1. D.L. Donohue, Anal. Chem. 74, 2002, 28A -35A

O18 We Are What We Breathe - An Examination of Potential Bioavailability of Metals in Aerosols

Wijdan Malik, Graeme Spiers, J. Abedin

The air we breathe is an assortment of metal rich particulate matter ranging from submicron sizes to ten-thousand times that. Previous research has determined that the mining and smelting industries across the Sudbury area have contributed to the severe heavy metal contamination of the aquatic and terrestrial environments. More recent research has confirmed that some of the main metallic contaminants in the surface layer of the regional soils include, Cu, Pb, Fe, Ni and As. Ingestion of these metals is a possible health risk for humans through exposure pathways such as inhalation of either vapour phase metals or

airborne particulates. Bioaccessibility is the portion from the dust samples that is mobilized during digestion across the intestinal epithelium to reach the hepatic portal vein before passing through to the liver. Filters from the Willet Green Miller Centre, Sudbury, Ontario, HVAC systems were obtained. The dust was collected with a vacuum, split into to specific fractions (less than 38 μm , 38-105 μm , 105-500 μm , 0.5-1 mm, 1-4 mm and greater than 4 mm) and characterized by combination of digestion and elemental analysis, Laser Particle Sizing, and scanning electron microscopy. The fine dust particulates (105 μm and less) was then subject to an environmentally controlled *In vitro* Gastrointestinal Digestion Model in which samples are subjected to simulated saliva, gastric juice, duodenal juice and bile juice, to create an extract for analysis. The extract was analyzed for total metal concentration using Inductively Coupled Plasma Atomic Absorption Spectrometry (ICP-AES). The concentration represents the bioaccessibility of the metal, and is compared to concentration standards set by health organizations. Overall 27 elements were quantified including metals As, Co, Cu, Fe, Mg, Pb and Zn. Results show significant bioaccessible amounts of Al, Cu, Fe, Mg, Ni, Pb and Zn in the dust. The results also, show trace bioaccessible amounts of Ba, Co, Cr and Mn.

O19 Challenges and Solutions for the Analysis of Pharmaceuticals and Personal Care Products in Environmental Samples

Chris Metcalfe, Shaogang Chu, Hongxia Li

PPCPs that are not rapidly degraded in sewage treatment plants (STPs) may remain dissolved in the aqueous phase of sewage effluents, or they may bind to biosolids. The most direct route of release of PPCPs into the environment is through the discharge of STP effluents into surface waters. Biosolids containing PPCPs may be placed in landfills or spread on agricultural land for soil amendment, where these compounds may be transported by runoff into the surrounding surface water or may leach into underlying groundwater. The most widely used method for analyzing PPCPs in environmental matrices is liquid chromatography with tandem mass spectrometry (LC-MS/MS). However, there are several analytical challenges associated with the use of LC-MS/MS instrumentation, including “matrix effects” that either reduce or enhance the signal as a result of co-extractives in the sample matrix. The electrospray (ESI) ion source is susceptible to ion suppression and our recent studies have shown that atmospheric pressure chemical ionization (i.e. APCI) is most susceptible to signal enhancement. Analytical solutions to these challenges include effective clean-up of extracts, use of low injection volumes, and calibration using “standard additions” methods or stable isotope surrogates. These methods have been applied to the analysis of PPCPs in complex environmental matrices, including the analysis of serotonin reuptake inhibitors in fish tissues and the analysis of beta-blocker drugs in both municipal wastewater and biosolids.

O20 Composition of Secondary Organic Particulate Matter from the Photo-Oxidation of Hydrocarbons Using APCI/MS-MS

Julie Bennett, Janeen Auld, Donald Hastie

An online system has been developed for the analysis of secondary organic particulate matter from the hydroxyl radical initiated photo-oxidation of hydrocarbons. It consists of a flow reactor, where particles and gases are produced, a Diffusion Denuder for gas/particle separation and an APCI MS-MS (TAGA 6000E) for composition analysis. The greatest challenge with this system has been to develop a method to quickly and efficiently isolate particles from the gases. The Diffusion Denuder is based on a denuder built by another research group (Ruiz et al., Harvard School of Public Health). It consists of three stacked channels separated by a polytetrafluoroethylene (PTFE) porous membrane. A sample flow consisting of gases and particles is introduced into the center channel, while pure air is sent to the upper and lower channels in a counter flow. Gases passing down the center channel will diffuse through the PTFE membrane into the upper and lower channels and be swept away to waste. Only particles will remain in the center channel since their diffusion coefficients are greater than the gases. The particles then can be directly sent to the TAGA 6000E for analysis. At this time gas and particle phase denuder characterization studies have been completed. The studies show that with a range of flow rates through the center channel, and upper and lower channels, gases are efficiently removed and particles are transmitted.

O21 Methylmercury Speciation in a Stratified Lake Using New DGT Sensors

Olivier Clarisse, Delphine Foucher, Holger Hintelmann

Speciation science seeks to characterize the distribution of an element among the various particular elemental and molecular forms in which it can exist in the environment in order to understand the transformations between forms which occur, and to infer the likely consequences – toxicity or biological activity – for the purposes of risk assessment. The major challenge of speciation analysis is the isolation, separation and quantification of the species leaving the original compound intact, which may be in some kind of equilibrium state with other species present in the sample. Mercury speciation analysis is a perfect example of this. The most toxic form of mercury, monomethylmercury, is an organometallic compound that exists in aquatic systems completely out of equilibrium with the other inorganic Hg species that are present. At the same time, within aquatic systems, methylmercury undergoes coordination reactions with a variety of ligands (chloride, sulfates, thiols molecules, fulvic and humic substance...) that approach equilibrium and which ultimately control its bioavailability. The Diffusive Gradient in Thin Films technique (DGT), recently developed by Davison and Zhang for *in situ* determination of kinetically labile metal species in aquatic systems, has been successfully used to monitor labile dissolved methylmercury in a stratified lake. DGT results have been systematically compared to independent measurements of the total dissolved concentration in order to investigate methylmercury speciation. Features and limits of this new sensor will be discussed.

O22 Thin Layer Chromatography Interfaced to Pyrolysis- GC/MS: Analysis of Crude Oils

Bob Helleur, Sandra Estévez

Advances towards the on-line coupling of thin layer chromatography (TLC) to GC/MS using a vertical furnace pyrolyzer as an interface has been described in a previous paper involving the analysis of the fatty acid composition of lipid TLC bands. This presentation will describe an environmental application of TLC-Py-GC/MS, the analysis of complex hydrocarbon fractions of crude oils, including the high boiling asphaltenes. Experiments involve the separation of crude oil using Chromarod TLC (15 cm x 1.0 mm; 5µm silica on quartz rod) into its four major bands, i.e., saturates, aromatics, resins and asphaltenes. The developed TLC rod is then inserted into a vertical furnace pyrolyzer and the individual hydrocarbon bands sequentially thermally-desorbed, or, pyrolyzed at 500 °C (for resins/ asphaltenes). The hydrocarbon products are separated and identified using high resolution GC/MS. Modifications to the pyrolyzer and GC interface, and, the experimental conditions will be described whereby the full length of the 15 cm TLC rod can be inserted and successfully scanned. Six different crude oils and one weathered (degraded) oil sample were analyzed. The oils could be chemically-differentiated (unique fingerprints) from one another by the partial mass chromatograms of their dibenzothiophene markers produced as the result of pyrolysis of the asphaltene band. Oils were further discriminated using chemometric analysis of dibenzothiophene and other hydrocarbon data.

O23 Exploring Chirality and Chiral Recognition Using Spectroscopic and *ab initio* Methods

Yunjie Xu

Chirality and chiral recognition are essential for living systems and are of great importance in the life sciences. We use experimental spectroscopic and *ab initio* methods to quantitatively characterize the phenomena of chirality and chiral recognition. I will first present the designs and constructions of three infrared spectrometers for such studies¹. I will then discuss a series of high resolution spectroscopic studies of molecular complexes of propylene oxide with common solvents, such as water and ethanol, and with itself². Using the experimental data, complemented with the *ab initio* calculations, we establish the structures and stability ordering of the complexes and examine the chiral discriminating forces at play in these molecular systems. The second part of my talk focuses on the effect of solvent-solute hydrogen-bonding on the vibrational circular dichroism (VCD) spectrum of methyl lactate. Some vibrational bands of an achiral molecule showed significant VCD strength through hydrogen-bonding to a chiral molecule. This effect, termed chirality transfer, will be discussed³.

1. W. Tam, I. Leonov, and Y. Xu, Rev. Sci. Instrum. **2006**, 77, 063117; Z. Su, W. Tam, and Y. Xu, J.

Chem. Phys. **2006**, 124, 024311.

2. Z. Su, N. Borho, and Y. Xu, J. Am. Chem. Soc. **2006**, 128, 17126; Z. Su, Q.Wen, and Y. Xu, J. Am. Chem. Soc. **2006**, 128, 6755; N. Borho and Y. Xu, Angew. Chem. **2007**, 119, 2171, 2326; Angew. Chem. Int. Ed. **2007**, 46, 2276. (VIP).

3. M. Losada and Y. Xu, Phys. Chem. Chem. Phys. **2007** (in press).

O24 The Scientific Contributions of ICP-MS

Sam Houk

A quick overview of the general scientific value and uses of ICP-MS will be presented. New developments in the following areas will be described: 1. Identifying the origins of polyatomic ions. 2. Reducing matrix effects and polyatomic ions by variations in sample introduction. 3. Controlled dissolution of surface layers for depth-resolved analysis.

O25 Significant Milestones in the Development of ICP-MS: A Manufacturer's View of the Growth of ICP-MS from a Research Device to a Mature Instrument for Routine Analysis

Fergus Keenan

ICP-MS has come a long way since Alan Gray built the DCP-MS in ~1971. Significant landmarks include the first ICP-MS spectra obtained by Alan Gray and Alan Date in 1981 and the first commercial orders placed in 1984. Rapid developments in technology ensued, driven largely by customer demand and robust competition between the primary vendors; VG and Sciex. Users were quick to adopt alternate sample introduction devices, some successful like Laser Ablation and some less fruitful like ETV. The development of tools like guard electrodes, high resolution and collision/ reaction cells broadened the appeal of the technique and opened up ICP-MS to a myriad of routine applications. By the late 1990s ICP-MS had become widely accepted as a routine tool for elemental analysis. This paper will review the significant developments in ICP-MS technology. The current state of the art including laser ablation, elemental speciation and collision/reaction cells will be presented along with a breakdown of what markets ICP-MS serves and how it has been implemented for a range of applications including geochemical, environmental, semiconductor and forensic analysis.

O26 ICP-Cell-MS; Norm or Exception?

Kaveh Kahan

Two landmark publications in 1989 demonstrated the potential use of radio-frequency-driven multipole collision cell in combination with inductively coupled plasma mass spectrometry (ICP-MS) for promoting ion-molecule reactions. However, it was not until a few years later that the collision and reaction cell technology was recognized as a viable approach by the major manufacturers, to resolve one of the challenges in ICP-MS, i.e. the spectral interferences. Since then, the rising demand for lower detection limits for all elements, particularly by the semiconductor industry, has resulted in an exceptional growth of the cell-based instruments in the field and the cell-based ICP-MS has become the method of choice in inorganic analysis, gradually replacing the traditional ICP-MS. In this presentation, the history and design of cell technology in inorganic analysis is reviewed and the key milestones that define the current state-of-the-art are identified. Also, the similarities and fundamental differences between the collision cell technology and the reaction cell approach are contrasted.

O27 The Collision Reaction Interface - A Simple Approach to Interference Management in ICP-MS

Doug Shrader, Shane Elliott, Xue Dong Wang, Iouri Kalinitchenko

Management of polyatomic and mass interferences in ICP-MS has been a popular area of research and topic of discussion in recent years. A novel interference management system for ICP-MS, the Collision Reaction Interface (CRI), will be discussed during this presentation. This unique technology employs simple collision and reaction gases injected directly into the plasma through the tips of the ICP-MS

interface cones. This approach quickly and effectively reduces or eliminates common interferences on elements such as As, Se, Cr, V and Fe, achieving lower detection limits in hot plasma, even for samples with complex matrices. Coupled with revolutionary 90-degree reflecting ion optics and a low noise, double off axis quadrupole mass analyzer, the CRI-ICP-MS offers an efficient yet simple solution to interference management in ICP-MS. The design of this unique CRI-ICP-MS will be discussed, along with principles of operation, performance attributes and application examples.

O28 Effect of a Pre-evaporation Tube on Arsenic Speciation Analysis

Shulan Liu, Diane Beauchemin

Because the toxicological properties of arsenic depend on its chemical form and its oxidation state, speciation analysis must be carried out to determine the types and the amounts of arsenic compounds present. The present work focused on four arsenic species, As(III), As(V), MMA and DMA i.e the most toxic ones. Their speciation analysis was accomplished using anion exchange chromatography, with inductively coupled plasma mass spectrometry (ICP-MS) as a detector. Baseline separation could be achieved using a simple concentration of ammonium nitrate at pH 8.6. The effect of inserting a pre-evaporation tube between the spray chamber and the torch was then studied. This heated tube preserves plasma energy by pre-evaporating the solvent before it enters the plasma, which allows an increase in the degree of ionisation of analytes with high ionisation potential, such as As, and thus significantly improved sensitivity. Furthermore, because this tube also decreases the aerosol droplet size distribution, which reduces noise in the plasma, it improved the detection limit even more. This improvement was, however, only observed for ionic species, because non-ionic analytes did not favour Coulomb explosions during sample evaporation. However, the enhancement could be generalised to all As species by adding concomitant analytes through a tee inserted between the chromatographic column and the ICP-MS detector. This indeed ensured that Coulomb fission events would still occur even when non-ionic analytes were eluting. This simple approach, which should be applicable to all ICP-MS instruments, should significantly enhance speciation analysis in general (i.e. not just for As).

O29 Clinical ICP-MS for Biomonitoring and Chemical Terrorism Preparedness

Michael Minnich, Amy Steuerwald, Patrick Parsons

The number of laboratories using ICP-MS to measure trace elements in biological samples is growing, especially among clinical laboratories that are transitioning from flame and electrothermal AAS methods. Among a network of established clinical laboratories, ICP-MS serves an increasingly vital function in biomonitoring and chemical terrorism preparedness. Currently, 62 jurisdictions which include all 50 states, 8 territories, and 4 major cities are part of a cooperative agreement with the U.S. Centers for Disease Control and Prevention to support these activities. The role that ICP-MS plays in the National Center for Environmental Health's Chemical Terrorism Response Program and the application of chemical terrorism resources to biomonitoring studies will be discussed.

O30 Screening Organophosphorus Nerve Agent Degradation Products by ³¹P ICP-MS

Joseph Caruso

Recent increases in terrorist activity and the threat of chemical weapon attacks has lead to the demand for a rapid and reliable method for analysis of chemical warfare agents (CWA) and their degradation products. The nerve agents Sarin and VX, as well as many others, pose a deadly threat to the human population if released. These phosphorus containing nerve agents along with their degradation products present difficulties for ultra-trace analysis due to their low volatility and lack of a good chromophore. Previous studies have successfully utilized methods such as gas chromatography/mass spectrometry (GC-MS), ion mobility/mass spectrometry (IMMS), and liquid chromatography/mass spectrometry (LC-MS) for the analysis of organophosphorus containing degradation products with detection limits in the ng/mL range. Chemical warfare degradation product analysis by inductively coupled plasma mass spectrometry (ICP-MS) coupled with ion-pairing reversed phase high performance liquid chromatography (IP-RP-HPLC) has recently been shown as a rapid and reliable speciation technique with detection limits in the pg/mL range. In this study the use of gas chromatography (GC) coupled with ICPMS detection is described for

the analysis of common degradation products of Soman, Sarin, Cyclosarin, Tabun, RVX and VX organophosphorus nerve agents. The developed method was successfully applied to complex river water and soil matrices. Clean separation from common P-containing pesticides is also shown.

O31 New Reagents and Instrument for Multiplexed Single Particle BioAssay with ICP-MS

Scott Tanner, Vladimir Baranov, Dmitry Bandura, Olga Ornatsky

The authors comprise the core of a multidisciplinary, multi-institute project to develop instrumentation, reagents and methods for the flow cytometric analysis of leukemic stem cells using tags designed for Inductively Coupled Plasma Mass Spectrometer detection. This presentation describes a new class of tagging reagent and a mass spectrometer detector for a novel flow cytometer that enables highly multiplexed measurement of many biomarkers in individual cells. The new instrument uses an Inductively Coupled Plasma (ICP) to vaporize, atomize and ionize the cell. The elemental composition, specifically of the tag elements, is recorded simultaneously using a Time of Flight Mass Spectrometer (TOF-MS). The detector provides for well-resolved atomic fingerprints of many elemental and isotopic tags, with little overlap of neighbouring signals (high abundance sensitivity) and wide dynamic range both for a single antigen and between antigens. A new class of tagging reagents, incorporating a reproducible number of transition elements (including the lanthanides and noble metals) has been developed and linked to antibodies: current sensitivity is 200 times greater for the application than commercially available products. We present the results of validation of the method-specific metal-polymeric tag reagents, DNA quantification through metalintercalation and gene detection using metal-tagged oligonucleotide probes. Experimental results showing multivariate biomarker response to cell line differentiation are presented, together with the first demonstration of multiplex analysis of single cells using the research prototype instrument.

O32 Has ICP-MS Delivered All it Promised?

Kym Jarvis

Twenty four years have passed since the launch of the first commercial ICP-MS instruments and the technique has truly reached maturity as have many of those early users! We have almost gone full circle – the original remit for the development of the technique being the requirement to find and exploit new uranium ore deposits to fuel a growing nuclear industry. Since then the tables have turned, and nuclear power industry in the UK became an almost taboo subject. In the last year however, this policy has taken an about turn and we are now seeing a renewed interest in all things nuclear particularly in the areas of new build materials and decommissioning. This presentation will take a look back at the early developments in the technique, major developments and the driving forces behind them. It will consider the bewildering range of applications to which the technique is now put as well as some recent applications in the author's laboratory: Has ICP-MS delivered all it promised – perhaps.

O33 Where ICP-MS Stands? A Manufacturer's Point of View

Chuck Douthitt

The sustained growth of the market for ICPMS has created a very competitive marketplace. The capital investments made by the instrument manufacturers has led only to many competing ICPMS technologies: the ICP source has been implemented onto virtually all possible analyzers (quadrupole, sector field, TOF, ion trap, Fourier transform, and Orbitrap). Quadrupole ICPMS (Q-ICPMS), with a market of ~ 750 units in 2006, dominates the market. The market is at present dominated by Thermo Scientific, Agilent, Perkin Elmer, and Varian. The second biggest technology is high resolution ICPMS (HR-ICPMS, a magnetic sector analyzer with a single collector), with a market of ~50 units in 2006, which is dominated by Thermo Scientific. Other commercially available technologies for elemental analysis include time of flight ICPMS (ICP-TOFMS), available from at least two companies, and ion trap ICPMS (ICP-ITMS) but the current markets for these two technologies are quite small. Multicollector ICPMS (MC-ICPMS, magnetic sector analyzer with a detector array), which is focused on high precision measurement of isotope ratios, and thus does not compete in the elemental analysis arena, had a market of ~15 units in 2006. This presentation will examine the tie ins of ICPMS with other optical technologies for elemental analysis, and

will acknowledge the profound debt that the manufacturers owe Professor Sam Houk, whose pioneering work is to be found at the base of much of the presently available instrumentation.

O34 ICP-MS – The Users Point of View

Don Chipley, Kurt Kyser

ICP-MS first used quadrupole mass analysers and sample introduction systems were limited to solutions. The field has evolved to include a diversity of instrumentation, including reaction and collision cells, magnetic sector ICP-MS, multicollector ICP-MS, and Time of Flight ICP-MS. Additionally, laser ablation was adapted for introduction of solid samples, followed by LC, GC and electrophoresis for chromatographic separations and speciation. Many applications of ICP-MS developed because of the unrivalled detection limits that are achievable, and presently include biology, geology, chemistry, biochemistry, forensic science, archeology and environmental science. We have used ICP-MS to investigate problems as diverse as mineral exploration using elemental concentrations in tree rings, measurement of trace metals in proteins, tracing of Bi in the environment and tracing of bird migration patterns. Additionally, multicollector ICP-MS offers the ability to measure isotopic ratios of a variety of elements that were not possible, or at least very difficult, by thermal ionization MS. Laser ablation measurements of U and Pb in uranium minerals reveal significant variations in U and Pb in minerals caused by partial resetting and gives insight into fluid and thermal histories of the largest features on earth, namely sedimentary basins. Time of Flight ICP-MS allows measurement of transient signals and quantification of small samples and has been applied to characterizing mineralizing fluids from single fluid inclusions. Sam Houk has contributed greatly to our understanding of ICP-MS. However, we, including Sam, must continue to investigate such problems as ion transmission and element and isotopic fractionations in the plasma and interface so that we can improve sensitivity and minimize isotopic and molecular interferences and isotopic bias.

O35 A Long-time User's Point of View on Where ICP-MS Stands

Diane Beauchemin

Since the first commercially-available inductively coupled plasma mass spectrometry (ICP-MS) instrument was introduced in 1983, the powerful features of ICP-MS were noticed, along with its limitations. Several subsequent developments in technology improved the technique's sensitivity and detection limit by numerous orders of magnitude. Collision and dynamic reaction cells as well as double focusing instruments have also been introduced to circumvent many spectroscopic interferences. However, one largely unresolved limitation remains, non-spectroscopic interferences, which arise from the sample matrix and can greatly complicate the analysis or degrade the precision of isotope ratios. During this presentation, several strategies that have been used over the years to alleviate this lingering problem will be reviewed. These include: sample processing approaches, from a simple dilution to matrix separation procedures ; calibration strategies ; instrument modifications, such as the addition of electrons proposed by Houk's group ; the use of a mixed-gas plasma ; and sample introduction strategies, such as chemical vaporisation and electrothermal vaporisation. Current knowledge on the sources of non-spectroscopic interferences will also be discussed. Space-charge effects can account for analyte signal suppression but not for enhancement. However, recent results obtained by the author's group indicate that a non-negligible source of non-spectroscopic interferences arises from the sample introduction system, which can result in either an enhancement or suppression of analyte signal. In particular, the matrix affects the number of Coulomb explosions, which can occur as aerosol droplets evaporate. The implications of this phenomenon will be considered.

O36 ICP-MS: As You Like It

Fred Smith

Almost 25 years have passed since the introduction of the first commercial inductively coupled plasma mass spectrometer (ICP-MS). Early quadrupole ICP-MS instruments allowed the selective and rapid measurement of many elements in liquid samples at ng/L levels and opened numerous new application areas. However, significant interferences on important elements (e.g. K,Ca,Fe) spurred much research for

interference reduction. So ICP-MS did not quickly progress to the Sixth Stage of an Analytical Method" of established applications. Other types of ICP-MS instruments were developed to markedly reduce interferences, such as high resolution ICP-MS and collision / reaction cell ICP-MS. In addition, advances in sample introduction and sample preparation provided enhanced analyte sensitivity, decreased interferences, and the ability to handle many sample types such as small volumes (< 1 mL) and even solids directly (e.g. laser ablation). Recent data will be presented using a nanoflow nebulizer (less than 500nL/min) for nanoHPLC coupled to ICP-MS. The use of nanoHPLC is important in bioanalytical studies when the amount of sample is only a few micrograms. The ICP-MS can be used to monitor heteroatoms in a biomolecule such as phosphorus, sulfur or selenium, providing complimentary data to electrospray MS/MS for proteomics. Overall, the variety of ICP-MS instruments available coupled with different sample introduction techniques provides for routine, specialized, and important new applications. For many users, ICP-MS can be "As You Like It".

O37 Modeling the Inductively Coupled Plasma: A Historical Review of Computer Simulations from Emission to Mass Spectrometry

Ramon Barnes

This presentation will trace the development and contribution of modeling and computer simulations of the inductively coupled plasma (ICP) for spectrochemical analysis from the 1970's to the present. Early representations were two-dimensional descriptions of the flowing ICP at atmospheric pressure, and contemporary models are four-dimensional including temporal variations. These models have helped to characterize the gas and particle flows, temperature and electron number densities, and droplet and analyte processes leading to spectrochemical signals and matrix effects in ICP discharges. Complementary experimental studies to verify model results and their correlations also will be described. ICP modeling status and some prospects will be considered.

O38 The ICP-MS Goes Environmental – Adventures With a New Toy

Graeme Spiers

O39 Industrial Applications of Calorimetry and Thermal Analysis

Charles Potter, Stewart Hunt

Physical and chemical properties are important to match the performance of industrial materials in many diverse applications. Thermal analysis and calorimetry provides critical information about the structure/property relationship of these materials, which aids in selecting the proper material for a specific end-use. TGA, DSC, MDSC[®], and microcalorimetry are used for the characterization of amorphous structure and the glass transition, quantitation of crystallinity, characterization of thermosets and cements, studies of thermal stability, and other physical properties.

O40 DSC-Microscopy: Seeing is Believing

Steve Sauerbrunn, Frank Palmisano, Bowen Greil

DSC has been the primary thermal analysis tool since its inception many decades ago. There are two main advantages of the DSC over DTA, the signal is quantitative in heat flow and the sample is encapsulated in a disposable aluminum crucible. There is no doubt that the quantitative heat flow is a big improvement over DTA and has led to the wide spread use of the DSC today. We did lose some information with the aluminum crucible. We cannot see the sample after the experiment as easily as we could when it was in a glass capillary used for the DTA experiments. Often, we cut open the crucible after the DSC experiment to see if the sample has changed such as: discoloration due to decomposition or weight change due to evaporation. If the sample did change during the experiment, we are left to ponder, 'Where in the DSC experiment did this change occur?' With the advent of low cost, high resolution CCD cameras, magnifying optics and windows it is now possible to record a video of the sample during the DSC experiment and retain the low noise, high quality DSC experiment. This technology is now offered with either the high pressure DSC or the standard DSC. It can be retrofitted onto any METTLER-TOLEDO

DSC. Applications will be shown that demonstrate the additional aid to interpretation that comes from recording a video of your sample simultaneously with the DSC experiment.

O41 Thermal Analysis Coupled to Online Evolved Gas Analysis

Elisabeth Kapsch, Peter Vichos

Thermal Analysis Coupled to Online Evolved Gas Analysis Dr. Elisabeth Kapsch Netzsch Instruments, Inc In Thermogravimetry (TG) or Simultaneous Thermal Analysis (STA), the mass change (and transformation energetics) of a sample versus temperature or time is measured. Evolved Gas Analysis (EGA) yields additional information regarding the nature (composition) of the gases evolved during a mass-loss step. The detection of gas separation and identification of the separated components are possible in exact time correlation with the other thermal analysis signals. In most cases, Quadrupole Mass Spectrometer (QMS) or Fourier Transform Infrared Spectrometer (FTIR) systems are coupled to a TG/STA system for evolved gas analysis. This is based on the fact that both EGA systems are fast methods. FTIR or MS spectrum can be measured within seconds. Therefore, the correlation with the mass loss step in the TG curve is ensured and can easily be done in the software. In addition, these methods are very sensitive, gas contents in the ppm-range can still be detected (QMS). A wide range of gas species can be detected with these methods and guarantee a broad application range. The following different coupling possibilities will be discussed in terms of techniques and advantages: • TG/STA-FTIR Coupling (Transfer Line) • TG/STA-MS Coupling (Capillary Coupling) • STA-MS Coupling (Skimmer) A wide range of application examples demonstrate the use of the hyphenated techniques in state-of-the-art research and development. In addition, an introduction into the PulseTA[®] technique will be given. With this technique an exactly defined quantity of gas or liquid is injected to the purge gas of the thermo-balance (TG) or the simultaneous thermal analysis instrument (STA). This clearly increases the measuring possibilities: the MS and respective FTIR signal can be calibrated. Separated gas quantities can be quantitatively determined with a precision of up to 0.01 %.

O42 The Matrix: Evolutions, Gaining Insight from Thermal Analysis

Pearl Lee-Sullivan

Polymers and polymer-matrix composites are becoming the mainstream materials in the manufacture of products for automotive, electronics, telecommunication packaging and aerospace applications. The selection and use of polymeric materials in engineering design is based on single point mechanical property data such as modulus or stiffness, yield strength and toughness. These properties are intimately linked to the polymer molecular structure which, however, evolve during processing and in-service. Since polymers are strongly viscoelastic, i.e. their properties are sensitive to time and temperature, it is possible to determine the rate and cause of mechanical property changes by measuring the intrinsic changes in time-temperature response. In this presentation, the use of thermo-analytical methods to characterize the viscoelastic response of thermoset and thermoplastic matrices will be illustrated. Thermo-mechanical methods detect molecular motion. They reveal the evolution of molecular-level readjustments as the polymer interacts with the changing environment, e.g. loading, temperature, moisture. A number of different research studies will be presented. One study shows how we may control the epoxy cure process to minimize process-induced stresses during adhesive bonding in aircraft patch repair. Another will show how stress relaxation data can be coupled with finite element simulation to explain moisture-induced adhesive failure in composite sandwich panels. For thermoplastics, it will be shown that the drastic changes in the mechanical properties (e.g. modulus, toughness loss) during the aging of high impact resistant polycarbonate can be directly correlated with microstructural rearrangements. Finally, the use of differential scanning calorimetry (DSC) enthalpic relaxation data to compare aging kinetics of polycarbonate with a blend of polycarbonate-acrylonitrile-butadiene-styrene will be presented.

O43 Cooling Rate Studies of a Polycarbonate/Acrylonitrile-Butadiene-Styrene Polymer Blend by DSC

Jacky Tang, Pearl Lee-Sullivan

The effects of cooling rate on a commercial polycarbonate and acrylonitrile-butadiene-styrene blend

(75:25 PC/ABS) has been studied using differential scanning calorimetry (DSC). The blend exhibits two distinct peak endotherms at about 90 and 110°C, which are associated with the glass transition of ABS and PC components, respectively. Cooling rate studies were performed on the unaged state of the material, as well as various aged states. The apparent activation energy for enthalpic relaxation for the unaged blend was found to fall between the activation energies for PC and ABS, respectively, but not according to the rule-of-mixtures. A main objective of the study was to compare the effects of cooling rate using the fictive temperature, T_f . By analyzing this rate of change in the fictive temperature, self-retardation behaviour was observed only at aging temperatures below $T_{g,ABS}$ (e.g. 80 and 90°C). However, aging 100°C did not show the same trend, as if the rate of change of fictive temperature was insensitive to aging time. This temperature lies between the T_g of the ABS and PC components, which suggests that the mechanism for structural relaxation in this range is very different from that of relaxation at sub- $T_{g,ABS}$ temperatures.

O44 Absolute Measurements of Thermal Conductivity of Acrylic Acid Solution by the Transient Hot Wire Technique

Feng Tian, James Venart, Ramesh Prasad, LiQun Sun

Absolute measurements of the thermal conductivity and the thermal diffusivity which are the important thermophysical properties of materials are of considerable significance to the industry and research work. The transient hot wire technique is now considered the most accurate method to measure the thermal conductivity of fluids. For the electrically conducting liquids, the coating technique has to be applied and becomes the leading method now. In this work, a new instrument is presented to measure the thermal conductivity and the thermal diffusivity of electrically conducting and polar liquids based on the tantalum wires with the tantalum pentoxide coating as sensing elements in the cell. The performance of the apparatus has been assessed by the measurements of propane which are compared with NIST.

O45 Raman Spectroscopy Resolution Limits Overcome by Sub-100nm Thermal Analysis

Roshan Shetty, Jiping Ye, Michael Reading, William King, Kevin Kjoller

Recently new sub 30nm micromachined thermal probes have become available that can obtain thermal properties at sub-100nm spatial resolution. Data will be presented of using these probes to study a blend of PA6 and PET and in this case it is shown how nanothermal analysis (nano-TA) can be used as a highly complementary technique with Raman microscopy. We show that the Raman study is limited by spatial resolution to 500nm and information below this size scale (ie sub-100nm) is obtained by nano-TA. By combining both techniques it becomes possible to visualize the highly complex morphology of this blend.

O46 DSC with the TGA/SDTA851e Taking Weight Loss into Account

Steve Sauerbrunn, Frank Palmisano, Bowen Greil

Heat flow measurements in a thermogravimetric measuring cell should also allow simultaneously measured changes in mass to be taken into account in the calorimetric result. To do this a temperature dependent adjustment factor is determined that converts the SDTA signal into a heat flow curve (DSC curve). The SDTA signal is the temperature difference between the temperature measured directly at the sample and the program temperature that serves as the reference. Analogous to the DSC, it indicates for example whether a decomposition process is exothermic or endothermic and shows in addition where phase changes or reactions with no change in mass occur. Another way to measure transition enthalpies is to determine the specific heat capacity (C_p) of samples. It is then better to perform the C_p measurement according to the sapphire method with isothermal intervals, which however means an interruption in continuous heating. In contrast to this, an adjustment curve allows the heat flow to be measured directly with SDTA at different heating rates and continuously over the entire temperature range without multiple measurements and without a comparison with sapphire. In this way, heats of reaction and phase transition enthalpies can also be determined by TGA/SDTA measurements even when changes in mass occur.

O47 Thermal Decomposition of Iron Compounds Modified by Hydrazine

Koyar Rane, Soubir Basak, Pratim Biswas

An improved particle size distribution was achieved in an online synthesis of nanosize iron oxides in a specially built furnace aerosol reactor (FUAR) by modifying the nebulized solvent soluble simple iron compounds by hydrazine. Further, it was observed that the precursors which otherwise yielded iron oxide of corundum structure, $\alpha\text{-Fe}_2\text{O}_3$, the modification lead to the formation of magnetic oxide of cubic spinel structure, $\gamma\text{-Fe}_2\text{O}_3$. In order to understand the mechanism for such formation of magnetic oxide, we investigated offline thermal decomposition of ferrous acetate, ferrous sulfate, ferric chloride, ferric nitrate ferrous/ferric acetylacetonate and ferrous oxalate and their hydrazine modifications. It was observed that hydrazine complexes, $\text{Fe}(\text{CH}_3\text{COO})_2 \cdot 2\text{N}_2\text{H}_4$, $\text{FeSO}_4 \cdot \text{N}_2\text{H}_4$, $\text{FeCl}_3 \cdot 3\text{N}_2\text{H}_4$, $\text{Fe}(\text{C}_5\text{H}_7\text{O}_2)_3 \cdot 1.5\text{N}_2\text{H}_4$, $\text{FeC}_2\text{O}_4 \cdot 2\text{N}_2\text{H}_4$ decomposed at much lower temperatures than the simple unhydrazinated compounds. The detailed thermal decomposition paths have been discussed in this paper.

O48 Thermoanalytical Properties of Wheat Gluten Protein Films

Subhash Mojumdar, R. Legge, C. Moresoli, L. Simon

Wheat gluten (WG) proteins can be utilized to make films with novel functional properties, such as selective gas barrier properties and rubber-like mechanical properties. WG-based materials are homogeneous, transparent, mechanically strong, and relatively water insoluble. They are biodegradable and biocompatible, and edible when food-grade additives are used and the presence of impurities is avoided. This review focuses on the possibility of replacing synthetic polymers with biodegradable polymers derived from renewable agricultural sources. WG films have been found to be very effective oxygen barriers. So, packaging applications that utilize the films' oxygen barrier ability are one possible area for WG film application. Several food items susceptible to lipid oxidation could benefit from multilayer packaging materials consisting of protein coatings in combination with an external moisture barrier. Protective protein coatings could also be used on certain food products, such as meat pies and high-moisture low sugar cakes that require films that are highly permeable to water vapor. Employing protein coatings as carriers of antioxidants and other food additives is another envisioned application. Protein films can also have application in implant medicine, biosensor design, food processing and chromatographic separation. Thermoanalytical techniques are valuable tools in the characterization of protein films. This presentation will review various thermoanalytical techniques such as TGA, DTA, DSC, MDSC and DMTA that have been applied to protein film characterization and identify their value and virtues.

O49 Kinetics of the Thermal Decomposition of Nitrocellulose

Daniel Martineau, Richard Turcotte, Barbara Acheson, Kelly Armstrong, Queenie Kwok

Nitrocellulose (NC) is the main ingredient of many gunpowder, explosives, and solid rocket propellants. Although much data exists on the kinetics of NC thermal decomposition, unexpected ignitions of NC based material are not uncommon, particularly during pressing operations on propellants. Historically, small-scale techniques have been used to study the decomposition of NC. These have produced a wide range of kinetic parameters applicable in different temperature ranges. The difficulty for the prediction of incidents involving NC based materials lies in proper translation of the results from small-scale experiments to manufacturing scales. Many models have assumed that the kinetics of NC decomposition is autocatalytic or first-order autocatalytic but convincing arguments have been given to the effect that two rate laws seem to be required to describe the decomposition process: first-order autocatalytic and simple second-order. In the present study, the kinetics of NC's thermal decomposition has been studied at the small scale by isothermal simultaneous thermogravimetry/differential thermal analysis (TG-DTA), coupled to FTIR and MS. The same was also studied by accelerating rate calorimetry (ARC), which is more representative of the manufacturing scale. A wide scatter in the deduced kinetic parameters is evidenced. The former not only depends on the experimental conditions, but also on the assumptions and models being used to derive these values. The measured values can be reconciled with other literature values through kinetic compensation considerations.

O50 Characterization of Polymeric Materials Using Laser-Induced Breakdown Spectroscopy (LIBS) and TGA, DTG and DSC

Subhash Mojumdar, M. Sain, Tulika Mojumdar

There have been exciting developments in laser sources, detectors, and optical instrumentation in the recent years. These new and increasingly portable sources have opened up series of new applications in laser-induced breakdown spectroscopy (LIBS). LIBS, also sometimes called laser-induced plasma spectroscopy (LIPS) or laser spark spectroscopy (LSS) is a useful analytical tool for determining the elemental composition of various solids, liquids and gases. High power laser pulse is focused on to a sample which creates plasma or a laser spark (breakdown). LIBS performs simple and rapid qualitative analysis and determines the elemental composition and the elemental concentration. Laser-induced plasmas were reported as early as 1962, shortly after the discovery of the ruby laser. They also enjoyed some attention in the 1960s as an analysis technique. Many progresses have been made during the last several years on the diverse and versatile applications of LIBS including space exploration, remote material analysis in nuclear power stations, diagnostics of archaeological objects and metal diffusion in solar cells, etc. The main advantages of LIBS compared to the conventional analytical spectrochemical techniques, such as inductively coupled plasma-mass spectrometry (ICP-MS), inductively coupled plasma-atomic emission spectrometry (ICP-AES), and graphite furnace atomic absorption spectrometry (GFAAS), are those of simplicity and speed. Little or no sample preparation is needed (sampling by laser ablation, high throughput and reduction of time consuming procedures). The characterization of various polymeric materials using LIBS, TGA, DTG and DSC will be discussed.

O51 Hydrazine Method of Synthesis of Al_2O_3 : Thermal Decomposition of Aluminum Carboxylates

Koyar Rane, Vrinda Borker, Manisha Shirodkar

In search of an easy way of formation of less agglomerated alumina at lower temperatures from precursor route we have been concentrating on hydroxides and carboxylates of aluminum. Carboxylates of metal ions are being extensively studied to synthesize metal and mixed metal oxides of technological significance. We have investigated the thermal decomposition of aluminum formate, acetate and oxalate. Formation of organo-aluminum hydroxide compounds of general formula, $M_n [R(COOH)_x]$ where, M is aluminum hydroxide, $Al(OH)_3$, n is in the range of 0.01 to 3.0 and is the number of moles of organic material reacted with a mole of M, R is an organic functional group having 0 to 15 carbon atoms and x is in the range of 2 to 4, has been discussed in an US Patent No. 5182410 (Filing date 12/14/1990). These hydroxides modified by carboxylates decompose giving novel alumina. We have synthesized $Al(HCOO)(OH)_2 \cdot 0.5H_2O$, $Al(CH_3COO)(OH)_2 \cdot 3H_2O$, $Al(C_2O_4)(OH)$. And then they are being further modified by hydrazination as, $Al(OH)_3 \cdot N_2H_4$, $Al(HCOO)(OH)_2 \cdot 2N_2H_4$, $Al(CH_3COO)(OH)_2 \cdot 0.5N_2H_4$ and $Al(C_2O_4)(OH) \cdot 1.5N_2H_4$. Thermal decomposition studies revealed the formation of alumina from hydrazine modified compounds at much lower temperatures as compared to the unhydrazinated ones. The detailed investigations of such systems have been discussed in this paper.

O52 Growth and Characterization of 2-bromo-4-chloroacetophenone (BCAP) Crystals

G. Madhurambal, P. Ramasamy, P. Anbusrinivasan, G. Vasudevan, S. Kavitha, Subhash Mojumdar

Non-linear optical (NLO) materials have wide applications in the field of telecommunication and optical information storage devices. The organic NLO materials play an important role in single harmonic generation (SHG), frequency mixing, electro-optic modulation, optical parametric oscillation and optical bistability, etc. Organic crystals have parameters superior to widely used crystals like KDP. 2-bromo-4-chloroacetophenone (BCAP) crystals were grown from carbon tetrachloride as solvent using slow evaporation technique at room temperature. Transparent, good quality BCAP crystals were successfully grown. Solubility studies were made using this solvent at different temperatures. Various functional groups present in the grown crystal have been identified using FTIR spectra. The grown crystals were also subjected to 1H -NMR and thermal analysis studies in order to confirm the structure and purity of the grown crystals. The transparency of the crystal was tested using UV-visible spectral analysis. The unit cell

dimensions of grown crystal were determined for the first time. Solubility and metastable zone width studies of BCAP in CCl_4 have been carried out at various temperatures.

O53 The Use of Insoluble Potato Fiber as a Microbial Carrier for Bioremediation

Mazen Saleh, Chris Elliot, Zhibin Ye, Subhash Mojumdar

We have investigated the basic physical properties of insoluble potato starch fibers to eventually evaluate its use as a matrix for binding/aggregating bacteria in bioremediation. Insoluble starch fibers were prepared from white potato (*Solanum tuberosum*) and sweet potato (*Ipomoea batatas*) and compared for their melting temperature by DSC and their ability to bind/aggregate bacteria. The DSC curve for white potato showed a maximal heat flow through the material at 127.34 °C (melting temperature of 105.09 °C). These numbers for the sweet potato fibers were 133.05 °C (101.42 °C), respectively. The two types of fibers, however, showed different binding/aggregation capacities for bacteria, with white potato approximately twice as many cells of *Burkholderia cepacia* (22.6 billion / g) as cells of *Pseudomonas putida*. The reverse was true for fibers from sweet potato, binding twice as many cells of *Pseudomonas putida* (23 billion / g) as cells of *Burkholderia cepacia*. Thermal analytical methods are found to be versatile in assessing the physical state and purity of these biological polymers. The TGA curves for both starches exhibited one main mass loss step corresponding to the DTG peak temperature at 323.39 and 346.93 °C, respectively.

O54 Synthesis of Nanosize Nickel Ferrite at Relatively Lower Temperature Using Novel Precursor Combustion Technique

Subhash Mojumdar, V. Verenkar, R. Nayak, A. More

Nickel ferrite is technologically important magnetic material extensively used in high frequency applications such as microwave device due to its high resistivity and sufficiently low losses. This paper reports the preparation of nanosized nickel ferrite by autocatalytic combustion of novel nickel ferrous fumarate-hydrazinate precursor. The part of this precursor, once ignited with a burning splinter under normal temperature and pressure conditions, glows and the glow spreads slowly over the entire bulk completing the autocatalytic combustion of the precursor to nanosized single phased nickel ferrite. The single phase formation of nanosized nickel ferrite was confirmed by XRD, IR spectra and HRTEM. The average particle size of the nickel ferrite was found to be ~20 nm, by TEM. The lower value of saturation magnetisation observed for nickel ferrite in the present study also confirms the nanosized nature of particles. The saturation magnetisation of the nanosized nickel ferrite increased with increasing sintering temperature up to 1000 °C, where it equals the reported value for the bulk nickel ferrite. The sintered nickel ferrite (1000°C/5hrs) was characterised by XRD, IR spectra, SEM, TEM, temperature variation of Resistivity, Seebeck coefficient and A.C. Susceptibility. The compiled results thus show that single phase nanosized nickel ferrite can be prepared at comparatively lower temperatures (~280°C) which can be sintered at relatively lower temperature and time (1000°C/5hrs) to achieve properties similar to the bulk nickel ferrite and still maintaining lower average particle size of 500 nm.

O55 Hydrazine Method of Synthesis of Al_2O_3 : Thermal Decomposition of Aluminum Hydroxides

Koyar Rane, Vrinda Borker, Manisha Shirodkar

Gibbsite, $\alpha\text{-Al}(\text{OH})_3$, is an industrially significant material being a major intermediate in the Bayer process for the extraction of alumina from bauxite. Gibbsite is an important precursor of alumina. The dehydration of gibbsite was studied extensively and is considered to be a complicated process as it passes through various metastable phase transformations (transition alumina). The transformations leading to $\alpha\text{-Al}_2\text{O}_3$ depend on the starting precursors and their preparation routes, heating environment, rate of heating etc. As our aim is to make use of the gibbsite from Bayer process ultimately to obtain uniform nanosize particles for practical applications, we are presently scanning the whole range of aluminum hydroxides synthesized from various laboratory chemicals as precursors for alumina to understand their thermal path of decompositions. Aluminum hydroxides, $\text{Al}(\text{OH})_3$, $\text{Al}(\text{OH})_3 \cdot 0.5\text{H}_2\text{O}$, $\text{Al}(\text{OH})_3 \cdot 1.5\text{H}_2\text{O}$, $\text{Al}(\text{OH})_3 \cdot 2.5\text{H}_2\text{O}$, $\text{Al}(\text{OH})_3 \cdot 3.5\text{H}_2\text{O}$, have been synthesized from commercial anhydrous AlCl_3 , $\text{Al}(\text{NO}_3)_3 \cdot 9\text{H}_2\text{O}$,

$\text{AlNH}_4(\text{SO}_4)_2 \cdot 12\text{H}_2\text{O}$ using NaOH and NH_3 as precipitants. The hydroxides have been further modified by hydrazination and the formation of a compound of a typical type, $\text{Al}(\text{OH})_3 \cdot 3\text{N}_2\text{H}_4$ has been established by chemical and infra red analysis.. It is found, in general, that the hydrazination enables the hydroxides to decompose at lower temperatures than that observed for the hydroxides. The decomposition path is, thus, altered by the hydrazination of the hydroxides. Thermal decomposition studies done on these have been discussed in this paper.

O56 TGA, DTA and UV, FTIR and NMR Spectral Characterization of Benzophenone and Mixed Crystal of BP and 2, 4 Dinitro Phenyl Hydrazone of Benzophenone

G. Madhurambal, P. Ramasamy , P. AnbuSrinivasan , M. Suganthi, G. Vasudevan , Subhash Mojumdar

Organic non linear optic (NLO) materials have greater importance due to their high non linear optical properties, rapid response in electro-optic effect and large second or third order hyper polarisabilities compared to inorganic NLO materials. In recent years considerable interest has developed in the study of organic compound exhibiting NLO properties. Benzophenone (BP) is one of such material. Good quality BP crystals were grown by solution technique using CHCl_3 as solvent by adopting slow evaporation method at room temperature. The grown crystals were subjected to various characterization studies to analyze its purity and applications. The condensation product 2, 4 dinitro phenyl hydrazone of benzophenone (DNPBP) was prepared by adopting standard procedure. Then mixed crystal of BP and DNPBP was grown by solution growth. Both the condensation product and mixed crystals were characterized using TGA, DTA, UV, FTIR and ^1H NMR. Thermal studies reveal the purity of the product. The second harmonic generation (SHG) efficiency of the grown crystals was determined.

O57 FTIR Spectroscopy and Thermal Analysis in Characterizing Various Materials

Tulika Mojumdar, M. Sain, Subhash Mojumdar

Fourier Transform Infra-Red (FTIR) spectroscopy often termed as IR absorption spectroscopy is a chemical analytical technique which detects the vibration characteristics of chemical functional groups in a sample. When a sample is IR-radiated, different molecules in the matter tend to absorb or transmit the incident IR light at different frequencies characteristic to those molecules only. It represents the molecular absorption and transmission, creating a molecular fingerprint of the sample. Generally, most functional groups tend to absorb above 1500 cm^{-1} . The region below 1500 cm^{-1} is known as the "fingerprint region". IR spectroscopy has become a useful tool for various types of analysis and is widely used to analyze inorganic and organic compounds in many industries including pharmaceuticals, chemical, petroleum, textiles, adhesives, food science, forensic laboratories and paper etc. Since, FTIR spectroscopy is a versatile technique which can be applied equally well to solid, liquid and gaseous matters, it employs a variety of identification methods suitable to the nature of the sample i.e. samples can be analyzed either using transmission or reflection spectroscopy which again can be subdivided into specular reflection, diffuse reflection (DRIFTS), attenuated total reflection (ATR) and IR reflection absorption (IRRAS). Generally the spectral bands appearing around 1630 and 3500 cm^{-1} are designated as those of water-vapor whereas CO_2 bands are characterized at around 667 and 2350 cm^{-1} . While taking IR spectra, one should always normalize it. FTIR spectroscopy can be used for qualitative as well as quantitative analysis. The use of various thermoanalytical techniques together with FTIR spectroscopy is the main aim of this contribution.

O58 Special Cement Blend Bound in Geosynthetics Liner: Application in Mechanical and Anti-rust Protection of Pipelines

Subhash Mojumdar, I. Janotka

Geotechnical products are divided into four main groups: textile mats, textile tubes, textile containers and filled – in textile liners. The last group is represented by geosynthetics clay liner (GCL) containing 8-mm thick mineral filler with bentonite filler usually. GCL is mainly used on the landfills as barriers preventing contamination of the surrounding environment. This paper describes technical innovation in which the standard GCL of Slovak provenance is replaced by a newly developed geosynthetics cement-based liner

(GCBL). Mechanical and basic geotechnical properties as well as chemical resistance and passivation ability of cement-based filler and behavior of GCBL with the above filler as the industrially-made product for mechanical and anti-rust protection of pipelines have been introduced. In the GCBL, mineral filler contains Portland cement as main component and 25 wt. % of additive providing a firm, voluminously stable and chemically resistant cement blend suitable for application in natural and engineering substrates. The results interpreted to date indicate that hardened cement-based filler when compared to reference Portland cement has lower expansion at similar values of dynamic and Young's modulus of elasticity and compressive strength, improved resistance to magnesium chloride and ammonium sulfate solution at the same passivation ability. Corrosion tests of steel in model soil electrolyte protected and unprotected by GCBL, and consequent cyclic corrosion tests of steel protected and unprotected in model soil electrolyte without and with cathodic protection show that GCBL with cement-based filler has the same anti-rust efficiency as that of cathodic protection. Present results support the idea of cathodic protection replacement by GCBL on steel pipelines in building applications.

O59 Oxygen Scavengers in Boiler Feed Water: Thermal Studies of Cobalt(II) 3,4 Diaminotoluene and Co(II) Diaminotoluene Hydrazinate Complexes

Koyar Rane, Sifali Bandodkar

Dissolved oxygen must be removed from boiler feed water if corrosion is to be prevented in the boiler material. Once the oxygen level is brought to < 10 ppm by standard methods, removal of the last traces of oxygen can be accomplished by treating the water with a reducing agent that serves as an oxygen scavenger. The use of hydrazine as an oxygen scavenger in boiler feed water is very common and well documented. Hydrazine in water reacts with dissolved oxygen producing gaseous N_2 and H_2O . The scavenging action of hydrazine is enhanced by adding an effective amount of trivalent cobalt complexes. Hydrazine solutions with cobalt (II) chloride and 3,4-diaminotoluene have been found to be suitable for the removal of oxygen. In order to know the scavenging action of hydrazine with such additives, we considered a possible formation of Co(II) complex with 3,4 diaminotoluene as, $[Co(C_7H_{10}N_2)_3]Cl_2$, and with hydrazine as, $[Co(C_7H_{10}N_2)_2(N_2H_4)]Cl_2$. As Co(II) complexes have been widely studied as dioxygen carriers and activators and cobalt complexed with diamino ligands found to form an adduct with oxygen, $(CoL_2)_2O_2$, we considered such a possibility of oxygen extraction from boiler feed water. Thermal decomposition studies of these cobalt complexes show an oxidative decomposition in the case of hydrazinated one and that may be the reason why scavenging of oxygen takes place. Results of such studies are being discussed here.

O60 Effect of Low and High Concentrations of KCl Dopant on ADP Crystals

G. Madhurambal, S. Meenakshisundaram, S. Parthiban, Subhash Mojumdar

The growth promoting effect (GPE) is observed with inorganic dopants like potassium chloride (KCl) and ammonium chloride (NH_4Cl) due to the complexation of trace metal ion impurities in solution. It was observed that organic additives like EDTA, urea and thiourea lead to an increase in the growth rate and improvement in quality of different crystals. The experimental results of the influence of low (1 M %) and high (10 M %) concentrations of potassium chloride (KCl) dopant on ADP ($NH_4H_2PO_4$) crystals are presented. The dopant results in an increase in the metastable zone width, leading to an enhanced crystal growth rate, at its low concentrations. In the presence of high concentrations of the dopant in the medium, the growth rate decreases appreciably. Further, low concentrations of dopant improve the crystalline quality with better transparency. The diffraction patterns reveal that there is no change in basic structure except for variation in intensity by doping. Slight broadening is observed in FT-IR peak of ADP in the $3500-3500\text{ cm}^{-1}$ range in the presence of high [KCl]. It appears that the dopant has not altered much the optical transparency of the crystal. SEM studies of pure and doped samples reveal that structure defect centers are formed in ADP crystals by the dopant. Second harmonic generation (SHG) efficiency measurements indicate that NLO property is enhanced appreciably by [KCl] dopant and the SHG is more pronounced at high concentrations. It seems that the molecular alignment of the crystal facilitates nonlinearity in the presence of the dopant. There are significant differences in DSC curves of pure ADP, and 1 and 10 M % KCl doped ADP.

O61 The Applications of Raman Spectroscopy and Thermal Analysis Characterization of Various Materials

Tulika Mojumdar, M. Sain, Subhash Mojumdar

When monochromatic light is passed through a sample most of the incident light is scattered elastically, a small portion is absorbed and gets lost in the process and a still smaller portion is scattered inelastically. This inelastic scattering of light which causes a change in vibrational and rotational energy of a molecule is called Raman Effect after the name of its discoverer Sir C.V. Raman who discovered it in 1928 and was awarded the Nobel Prize in Physics for the same in 1930. Raman spectroscopy analyses the Raman scattered light inferring much about the chemistry and physics of the material. Basically, Raman spectroscopy is a non-destructive chemical technique commonly used in chemistry to study vibrational information which is very specific for the chemical bonds in molecules. Therefore, it provides a fingerprint by which the molecule can be identified. The fingerprint region of organic molecules is in the range 500-2000 cm^{-1} . It is also used to study changes in chemical bonding, e.g. when a substrate is added to an enzyme. Raman spectroscopy is useful for analyzing molecules that do not have a permanent dipole moment and therefore would not show up on an IR spectrum. Raman spectroscopy can be used to determine bond lengths in non-polar molecules. It is useful for determining the identity of organic and inorganic species in solution, as the Raman transitions for these species are more characteristic than for IR, where the transitions are much more affected by the other species present in the solution. Both, Raman and IR spectra provide complementary information. Typical applications are in structure determination, multicomponent qualitative and quantitative analysis. The aim of this work is applications of various thermoanalytical techniques and Raman spectroscopy in various materials characterization.

O62 Synthesis, Characterization, Fungicidal and Bactericidal Activities of Metal Diethyldithiocarbamate Fungicides

Subhash Mojumdar, H. Rathore, K. Ishratullah, C. Varshney, G. Varshney

The plant protection has become necessary due to increase the food production. The group of dithiocarbamate is of special interest among the commercially available fungicides at present. Zinc dithiocarbamate (zineb, ziram), manganese dithiocarbamate (maneb), iron dithiocarbamate (ferbam) are well known fungicides which are used as protective fungicides in grapes, cauliflower, potatoes, chillies, apples, groundnut, paddy etc. for the last many years. Their effectiveness has somewhat reduced and their large doses are required for fungal control. Thus there is a growing interest in synthesizing new dithiocarbamates, which can be applied at low concentration to control the fungal growth. Therefore, Copper diethyldithiocarbamate, Cadmium diethyldithiocarbamate, Lead diethyldithiocarbamate, Nickel diethyldithiocarbamate and Zinc diethyldithiocarbamate have been synthesized. They have been characterized using DTA, TGA, IR and X-ray and Atomic absorption spectrophotometry. Their solubility in sodium hydroxide, mineral acids, organic solvents, distilled water and salts solution has been measured. Fungicidal activity of the dithiocarbamates has been tested by well or cup diffusion method using five fungi species. Their bactericidal activity has also been tested by broth dilution method using six bacterial species.

O63 Solution Grown Benzophenone: Study of the Thermal Properties, Nucleation Parameters, Induction Period and Interfacial Energy

G. Madhurbal, P. Ramasamy, P. AnbuSrinivasan, Subhash Mojumdar

Organic single crystals possess unique optoelectronic properties. Benzophenone is a well-known organic material, which exhibits non-linear optical (NLO) property. It has been grown by solution technique adopting slow evaporation method from solvents CHCl_3 , CCl_4 for the first time. Solubility metastable zone width and inductions periods of benzophenone in CHCl_3 and CCl_4 were determined. Interfacial tension values at two different temperatures for various super saturations, such as 1.10, 1.15, 1.20 and 1.25 were determined using induction period. From interfacial tension values, the nucleation parameters, such as the radius of the critical nuclei (r^*), the free energy change for the formation of a critical nucleus (ΔG^*) and the number of molecules in the critical nucleus were also calculated for benzophenone in CHCl_3 and CCl_4 at two different temperature. Its thermal property was studied using TGA and DTA.

O64 Thermal Analysis of 2-Oxocyclopentanedithiocarboxylato Complexes of Iron (III), Copper (II) and Zinc (II) Containing Pyridine or Morpholine as the Second Ligand

Ranjit Verma, Lata Verma, Manishi Ranjan, B. Verma, Subhash Mojumdar

A series of ternary complexes of the types $M_2L_1L_2L_3$; $ML_1L_2L_3$ (M=Fe,Cu,Zn; L_1 =2-oxocyclopentane dithiocarboxylate; L_2 =pyridine, morpholine) and $CuL_1L_2H_2O$ was prepared afresh. Except the iron complex, all are dimeric and complexation is through the dithio moiety of the ligand L_1 . Their thermal decomposition was carried out in air with heating rate programmed at 100C/ min and it revealed that the dehydration of the aquo complex follows the same path as the carboxylates¹ and the pyridine complexes have the tendency to follow one step decomposition. The copper complexes are less thermally stable. The overall thermal stability of the 2-oxocyclopentanedithiocarboxylato complexes of the three metals with the volatile ligands was found to be in the order: $(CuLmorph)_2 < CuL_2H_2O < (CuLpy)_2 < (ZnLmorph)_2 < (ZnLpy)_2$

ABSTRACTS – POSTER PRESENTATIONS

P01 Analysis of Polycyclic Aromatic Hydrocarbons (PAHs) using an Atmospheric Pressure Chemical Ionization Triple Quadrupole Mass Spectrometer

Elize Ceschia, Donald Hastie, Nick Karellas, Janeen Auld

As part of a program to investigate the use of mass spectrometry (MS) for PAH investigation, the MS and tandem mass spectrometry (MSMS) spectra of selected PAHs were examined. 2-methylnaphthalene, anthracene, pyrene and fluoranthene were admitted to an APCI triple quadrupole mass spectrometer. All species were ionized where both charge and proton transfer ionization were observed. Due to weak ionization conditions in the APCI source, little fragmentation of the PAH m/z peak was observed in the MS scan. The MSMS spectra, showed fragments of the parent ion which could be understood and used for further identification. For the isomers, pyrene and fluoranthene, the MSMS were essentially the same but the compounds could be separated by collision energy. It appears as if APCI MSMS can identify PAHs although more compounds need to be studied and sampling methods need to be developed.

P02 Variations in Mercury Stable Isotope Ratios in Low Level Environmental Samples

Delphine Foucher, Wang Zheng, Holger Hintelmann

Analytical advances in the past decade and the recent advent of multicollector inductively coupled plasma mass spectrometry (MC-ICP/MS) have made it possible to measure fractionation of non-traditional elements, where mercury is still one of the more uncommon elements to study. Mercury has seven natural isotopes (^{196}Hg , ^{198}Hg , ^{199}Hg , ^{200}Hg , ^{201}Hg , ^{202}Hg and ^{204}Hg). Because all seven isotopes are stable, any variation measured result from natural fractionation processes. In our group, we have developed a method for accurate and precise determination of Hg isotope ratios in a wide range of environmental samples. An on-line Hg cold-vapor technique, using stannous chloride as reductant, was coupled to a Thermo-Finnigan *Neptune* MC-ICP/MS. All isotopic ratios were corrected for instrumental mass discrimination by simultaneously monitoring $^{205}\text{Tl}/^{203}\text{Tl}$ of a standard solution. Finally, variations of the isotope composition of Hg were determined relatively to a standard (Mercury Standard Solution NIST SRM 3133) using the standard-sample bracketing approach. Combined to a preconcentration technique, this method was employed to measure mercury isotope ratios in water and snow samples from Experimental Lakes Area (Ontario, Canada) and Ny-Ålesund (Spitzberg Islands, Norway). For the first time, mercury stable isotope compositions were determined for low mercury level samples ($< 10 \text{ ng L}^{-1}$).

P03 Novel Method for the Study of the Distribution of Metal and Metal-Complexes in Aqueous Slurries of Sediments

Meher Chowdhury, Marc Lamoureux

A novel method is being developed to study the distribution of metal and metal-complexes in aqueous slurries of sediment. This method was developed to study aqueous metal ions (e.g., Cu^{+2} and Pb^{+2}) in contact with an organic acid (e.g., EDTA) and model sediment, under controlled environmental conditions (temperature, pH, etc.). The method combines a high performance liquid chromatographic (HPLC) method with UV-detection and/or ICP-MS measurement. In addition, a micro-extraction cell is added prior to the analytical column that allows the direct injection of whole slurries into the analytical system. The method involves separation by ion-exchange chromatography on a reversed-phase C18 column coated with ion-pair reagent. The method uses a micro-extraction cell, which allows whole sediment slurry (suspended sediment) in contact with metal ions and organic acid to be injected, on-line, into an HPLC coupled to an ICP-MS. This arrangement allows temporal (chromatography) and mass (mass chromatography) separation of different metal species (free and bound to ligands). This unique approach can provide thermodynamic and kinetic information (e.g., equilibrium constant and sorption/desorption rate constant) on complex, environmental system. Results from a model system made of a Cu^{2+} - EDTA solution in contact with a model sediment will be presented and discussed.

P04 Mercury (Hg) Isotope Fractionation during Bioaccumulation in Aquatic Food Webs

Mark Dzurko, Delphine Foucher, Holger Hintelmann

Measurements of the natural fractionation of mercury (Hg) isotopes are a powerful tool to directly identify biogeochemical processes controlling the fate of mercury in the environment. In this study, we will investigate the possibility for Hg isotopes to undergo biological fractionation during bioaccumulation in a range of aquatic food webs. Initial work has been conducted to investigate a viable extraction technique that will separate mercury species from various biotic matrices. The selected technique permits the separation of the two most abundant forms of Hg in natural waters and biota - monomethyl Hg (CH_3Hg^+) and mercuric Hg (Hg^{2+}) - on the basis of the difference in charge of their respective thiourea ($\text{S}=\text{C}(\text{NH}_2)_2^0$) complexes. A cartridge containing thiol-functionalized silica resin will trap Hg^{2+} and CH_3Hg^+ from prepared sample solutions without retaining interfering sample matrix components and will be capable of eluting the Hg species without the need for any further chromatographic separation. An on-line Hg reduction technique using stannous chloride as the reductant will be applied for accurate and precise mercury isotope ratio determinations by Multi-Collector Inductively Coupled Plasma - Mass Spectrometry (MC-ICP/MS). Aquatic ecosystems containing point-source contamination of Hg may exhibit isotope signatures that reflect the input source and could potentially be traceable in their respected food webs.

P05 The Application of DRC Technology to the Removal of Polyatomic Interferences During the Analysis of Precious Metals in Geological Samples by ICP-MS

Chantal Blanchard, Oliver Burnham

A number of significant polyatomic interferences are known to impede the routine analysis of precious metals in geological samples via ICP-MS. Some of the predominant interferences arise from the formation of oxides by high field strength elements (HFSE: Zr, Nb, Hf, Ta and W). Dynamic reaction cell technology has been shown to significantly attenuate such oxide interferences by using oxygen as a reaction gas. However, routine precious metal analysis in geological samples remains a challenge. Such samples generally possess complex chemical compositions that lead to a large range of potential polyatomic interferences. In addition to the HFSE oxides, these include base-metal argides and/or REE chlorides. Furthermore, in most geological samples, there is expected to be a large contrast in concentrations between analytes and interfering elements. In order to establish a method for the determination of precious metals after a conventional acid-digest, the applicability of an oxygen-based DRC technique was investigated in more detail. Whereas the NbO, TaO, and WO interferences on Ag, Au, and Pt were found to be successfully removed, substantial amounts of ZrO and HfO were found to remain, limiting the capacity of the technique for the analysis of Pd and Pt. Based on the reaction profiles of these HFSE oxides and other polyatomic interferences, the range of samples to which the method can be applied will be presented.

P06 Mineralogical Controls on the Response of Geological Samples to Aqua Regia Leaching

Oliver Burnham

Although strong acid leaches (e.g., aqua regia) are commonly used for the determination of base and precious metals as part of regional or localised mineral exploration programs, the effect of such acids on common rock-forming minerals and accessory phases appears to be poorly understood by many in the exploration community. In order to investigate the effect of mineralogy on the susceptibility of different elements to aqua regia extraction, the mineral compositions from a suite of mineralised and non-mineralised samples were determined using scanning electron microscopy before and after acid attack. These experiments confirmed that the compositions of many oxide and silicate minerals appear to remain unaffected by aqua regia attack but that most common carbonates, base-metal sulphides, arsenides, and tellurides are completely digested. However, there do appear to be a number of exceptions to this general rule that need to be considered when presenting or interpreting aqua regia data. Of particular note are the leaching behaviours of Mg-Fe orthosilicate (olivine), REE phosphates (monazite and xenotime), and diverse precious metal minerals (Pt, Pd, Rh, Ir, and Ru sulphides, tellurides, arsenides, and antimonides). The results of the experiments will be presented and their significance discussed.

P07 Application of Different Analytical Techniques for Determination of the Cesium Distribution in High Burnup Fuel Samples

Andrei Izmer, Stefano Caruso, Niko Kivel, Renato Restani, Matthias Horvath, Ines Günther-Leopold

The determination of the migration of volatile fission products like cesium and thus an estimation of the rates of release are important criteria for the integrity of irradiated fuel rods from nuclear power plants. Different analytical methods are used in post-irradiation examinations to ensure the product quality of reactor core components and to provide data for nuclear safety approval procedures. The non-destructive technique of computerized tomography (CT) was applied on high burnup fuel rods for the determination of the within-pin distribution of fission products like cesium and europium. To perform such investigations, a high resolution gamma-ray spectrometry measurement station, allowing transmission and emission tomography, has been built. The results of this technique indicated a large depression in the cesium distributions at the centre of the pin, with higher concentrations in the peripheral region. In order to support these data, other analytical techniques were applied on samples from the same fuel rod. Electron probe microanalysis (EPMA) analyses have been performed to gain information about the elemental distribution of cesium and other elements (actinides and fission products). In order to obtain information about the isotopic composition the combination of a laser ablation system with an inductively coupled plasma mass spectrometer was used as a complementary analytical method. The interpretation of the measured data on the solid fuel samples was supplemented by HPLC-MC-ICP-MS measurements on fuel solutions from the same fuel rods. The presentation will compare the results from the different analytical techniques and discuss the advantages and limitations of each of them.

P08 Method Development for the Extraction of Volatiles from Molds by SPME-GC/MS

Don Parkinson, T. Churchill

This poster details the development of a preparative sampling and analysis method using solid phase microextraction (SPME) coupled to gas chromatography-mass spectroscopy for the elucidation and identification of out-gassed volatiles from molds in buildings. Methyl benzoate, a typical out-gassed analyte, was used as a model compound for method parameter optimization. The process of optimizing is outlined, and the results obtained from both spiked surrogate samples and real samples containing a variety of mold volatile organic compounds (MVOC) and mold metabolites are compared. The marriage of such "green chemistry" sampling methods to a selective separation and detection technique is discussed. Further its potential application to onsite monitoring and sampling schemes is also assessed.

P09 Trace Metal Content in Atmospheric PM_{2.5} Collected in Selected Canadian Locations: from Sampling to Analysis and Data Interpretation

Valbona Celo, Ewa Dabek-Zlotorzynska, David Mathieu

Atmospheric fine particulate matter of 2.5 μm or less in diameter (PM_{2.5}) plays a key role in climate issues and health problems. For this reason, a great deal of research has focused on the chemical characterization of atmospheric PM, including heavy metals, most of which are toxic to humans and ecosystem. This work presents data on the analysis of over 800 PM_{2.5} samples collected at selected rural and urban sites within the Canadian National Air Pollution Surveillance network. Integrated twenty-four hour PM samples were collected using a one-in-three day schedule from May 2004 to September 2006. Trace metal concentrations were determined using two independent methods, a non-destructive energy dispersive XRF method and an ICP-MS method with near-total microwave assisted acid digestion. Results obtained by both methods compare very well, confirming that the digestion method accomplishes the dissolution of metals with high recovery (>70%) depending on the metal. Although the ICP-MS method requires the digestion of samples, its low detection limits allow reliable quantification of a higher percentage of samples for the presence of various metals (e.g. V, Ni, Mn, As, Se, Sn, Sb, Pb) in comparison to the XRF method. Thus, the ICP-MS results were used for further data interpretation. Various multivariate statistical methods were applied in order to assess the impact of relevant sources and the meteorological factors at the sampling sites. The obtained results will be discussed.

P10 Bioaccessibility of Transition Metals in Airborne Particulate Matter

Jianjun Niu, Pat Rasmussen, Marc Chenier

Metals present in particulate matter have been implicated in a variety of cardio-respiratory illnesses associated with exposure to urban air pollution. Transition metals (e.g., V, Cr, Fe, Mn, Co, Cu, and Zn) receive particular emphasis due to linkages between oxidative stress and impaired lung function. In this study, size fractionated samples of indoor and outdoor urban particulate matter were collected on Teflo™ filters. For total metal determination using ICP-MS, digestion using ultrasonication in a strong HF-HNO₃ acid mixture was selected as the optimum approach for handling large numbers of filter samples while at the same time minimizing the risk of sample contamination. Two buffered extraction methods, ammonium acetate (pH 7; 0.01 M) and ammonium citrate (pH 5; 0.1 M), were compared with a simple deionized water extraction to evaluate the most appropriate approach for assessing metal bioaccessibility (the soluble metal concentration in dust particles expressed as a percentage of the total metal concentration). Comparisons using a series of NIST Certified Reference Materials and urban dust samples showed order of magnitude results between the methods, which appear to be pH and complexation related. A trial run using size-fractionated samples of PM trapped on Teflon™ filters indicates that the ammonium citrate extraction is most likely to yield metal concentrations that exceed method detection limits for low-flow 24-hr personal exposure samples.

P11 Single-run ICP-MS Analysis of Major Cations, Phosphorous and Trace Metals and Heavy Metals in Natural and Waste Water Samples: QC/QA Protocol and Methodology Considerations

Howard MacDonald, Marc Lamoureux, Darryl MacPherson, Shauna Thompson

This presentation will report on the possibility of performing, in a single run, the quantitative, accurate chemical analysis of several parameters such as major cations, phosphorous, and heavy metals in natural water and wastewater samples. The single-run, multi-parameter chemical analysis is conducted on an inductively coupled plasma mass spectrometer (ICP-MS) equipped with a special sampler/skimmer cones interface (Xi interface™, Thermo Elemental). This special interface allows the high concentration major cations (e.g., Na, K, Ca, and Mg) to be analyzed together with trace level metals (e.g., As, Cd, Pb, and U) during the same run. Details on the experimental methodology will be presented and discussed. In addition, a rigorous Quality Control (QC) and Quality Assurance (QA) protocols have been developed to ensure results accuracy for different type of water samples. The QC protocol includes a series of reference materials that are very diverse in chemical nature. For example, lakewater spiked with various analytes such as phosphorous, trace metals and major cations are routinely used, as well as wastewater samples to assess repeatability (duplicate) and matrix interference (spike recovery). The QA protocol includes a specially adapted performance report with key indicators of performance and the participation in proficiency test (PT) coordinated by Canadian Association for Environmental Analytical Laboratories (CAEAL) and National Water Research Institute (NWRI). Examples of proficiency testing will be presented and discussed.

P12 Arsenic, Selenium and Indium as the Fingerprint of Smelter Contamination in Ombrotrophic Peats of the Sudbury, Ontario, Region

Lizane Pamer, Oliver Burnham, Graeme Spiers

The use of ombrotrophic peat as an archive of atmospheric pollution has the potential for the unique differentiation of multiple and complex contamination influx sources. Industrial processes releasing fly ash, dust and particulates to the atmosphere have individual emission signatures that are largely dependent on the chemical make-up of diverse combustion materials and processes. The smelting of copper- and nickel-rich ores can release a suite of elements that includes arsenic, selenium, indium and lead in the process dusts and smokestack plumes, and with atmospheric transportation and subsequent deposition over time and landscape, can leave behind a historical fingerprint of pollution. Three ombrotrophic peat cores were collected from locations within 100 km of smelting operations in Sudbury, Ontario, and examined as potential archives of anthropogenic deposition. Each core exhibits arsenic, selenium, and indium enrichments that coincide with high concentrations of smelter-derived base metals. The As-Se-In

elemental ratios within these enriched zones resemble those of Sudbury ores, indicating that Sudbury smelter activities may have been a dominant source of contamination. $^{206}\text{Pb}/^{207}\text{Pb}$ isotopic ratios within the peat cores indicate additional contribution(s) from one or more anthropogenic sources at each site.

P13 Determination of Selenium by HG-ICP-DRC-MS in the Brain Tissues of Laboratory-raised Mink Dosed with Selenium and Mercury

Eavan O'Connor, Doug Evans

Selenium (Se) has been correlated positively with total mercury (THg) in various animal tissues, particularly with increasing proportional inorganic Hg. The mechanisms of co-accumulation are unknown but it is important to understand these processes because Se may mitigate methylmercury (MeHg) toxicity. The purpose of the present study is to develop a suitable method for the determination of Se concentrations in brain tissue of mink using HG (Hydride Generation)-ICP-DRC (Dynamic Reaction Cell)-MS after multistage microwave digestion and hot acid reduction. Sets of mink were fed diets spiked with different concentrations of Hg and an elevated but constant Se concentration with the objectives of 1) observing the strength of the correlation between Hg and Se in the brain and 2) determining if the proportions of Hg species (i.e., organic and inorganic) in THg differ according to Se concentration. Co-accumulation and an increase in the percent of inorganic Hg may mean that Se can detoxify MeHg in mink (although this situation does not imply detoxification). The Cold Vapor-Hydride Generation system will be used to purge volatile Se hydride from solution (4M HCl) using NaBH_4 as the reducing agent. Using this method, analyte transport efficiency to the plasma is maximized and matrix interferences are removed; therefore, recovery and sensitivity are increased while noise is decreased. Interferences from argon gas will be avoided by using ammonia as the cell gas in the ICP-DRC-MS. Potential problems include memory effects between samples and instability of the signal due to an excess of hydrogen produced during hydride generation.

P14 Mercury Isotope Fractionation during Volatilization of Hg(0) from Solution into the Gas Phase

Wang Zheng, Delphine Foucher, Holger Hintelmann

This work was to determine mercury isotope fractionation during volatilization of Hg(0) dissolved in aqueous solution to the gas phase and to develop a method for the precise determination of isotope ratios of gaseous Hg(0) by multicollector ICP/MS. Hg(0) was generated *in situ* by reducing Hg(II) using SnCl_2 and subsequently purged into a trapping solution. A $316 \mu\text{M}$ KMnO_4 , trapping solution, acidified by 0.9 M sulphuric acid recovered 0.961 ± 0.040 % of Hg (2 SD, $n = 20$). The observed $\delta^{202}\text{Hg}$ of -0.049 ± 0.065 ‰ (2 SD, $n = 17$) relative to the initial Hg standard, was not greater than the daily external precision of the isotope ratio measurement (< 0.1 ‰, 2 SD). The volatilization experiments were conducted by reducing Hg(II) completely using SnCl_2 , letting the developed Hg(0) evaporate from solution and purging the Hg(0) vapor in the headspace over the solution into the trapping solutions. The isotope fractionation during volatilization followed a Rayleigh fractionation with an observed maximum $\delta^{202}\text{Hg}$ value of 1.48 ‰ ± 0.07 ‰ (2 SD), and fractionation factors varying from 1.00044 to 1.00047. These results provide the first experimental proof for, and quantified the pattern and magnitude of the Hg isotope fractionation during volatilization of Hg(0) from solution into the gas phase.

P15 What Do Sequential Extractions Really Dissolve from Sediments – a XANES Study

John Hechler, Pamela Koski, Alan Lock, Graeme Spiers

Lake sediments form an archive for the concentration of both particulate and soluble aerosolic additions of the entire up-stream watershed basin. The current research project documents an investigation of the modern history of regional contamination as recorded within the sedimentary column of Ramsey Lake, Sudbury, Ontario, a lake at the centre of the airshed of the Sudbury basin. A seven-step sequential extraction was chosen to enable the determination of the proportion of metals bound to the various fractions within the Ramsey lake sediments. Reagents were chosen to solubilize the metals bound to the following specific fractions or phases of the freeze-dried sediments: exchangeable, acid-soluble, bound to organics, bound to manganese oxides, bound to iron oxides, bound to recalcitrant organics and sulfides,

with a residual fraction remaining. The specificity of each sequential extraction stage for sulphur and phosphorus compounds was examined by analyzing the sediment residue at each extraction step by X-ray absorption near edge structure (XANES) at the S and P K-edges. The resultant sulfur and phosphorous spectra suggest that the residue after each step remained essentially unchanged until the second last extraction step, with a subsequent mild oxidation producing a shift from sulfide to sulfate dominant phases in the residual sample. These preliminary observations imply that the reagents used to solubilize the organics did not oxidize the mineral phases within the original sample, whereas the reagents used to solubilize the recalcitrant organics and sulfides did perhaps lead to a negative enrichment of sulphate phases in the samples. The P K-edge XANES spectra are essentially unchanged after all chemical extractions, indicating that the selective chemical extractants do not effect any residual phosphate bearing mineral phases within the sedimentary column.

P16 Atmospheric Particulate Matter Within The Sudbury Footprint

Pamela Koski, Graeme Spiers

Measuring the chemical and mineralogical composition of coarse, fine and ultra-fine dust and their association with metals in the air is important for health and ecosystem risk assessments. Therefore, the determination of the concentration in the different particle size fractions which may exist in the atmosphere is essential. The goal of this study was to investigate the concentration, particle size distribution and spatial dispersion of metals in total and fractioned airborne dust. Samples of airborne dust were collected at five different sites over a one year period in the Sudbury area, including one control site located downwind of the south-westerly most industrial emission source. Sampling was performed simultaneously at all five sites to account for spatial distribution and atmospheric transport of metals. The total concentration of As, Co, Cr, Cu, Mn, Ni, Pb and Zn in dust samples was estimated using x-ray fluorescence (XRF). Data indicates that the sites within the City of Greater Sudbury contained the highest metal concentration, with the majority of the metals quantified residing in the respirable size fraction, PM_{2.5}. The examination of the S K-edge region, using X-ray absorption near edge structure (XANES), in the PM₁₀₊, PM₁₀-PM_{2.5}, and PM_{2.5} size fractions at three selected sites revealed that atmospheric S is mostly in the form of sulphate.

P17 Has the Signature Been Retained ... the Chemistry of Lakes Downwind of a Smelter Region, Sudbury, Ontario

Aimee Williamson, F. Prevost, Alan Lock, T. Maki, Graeme Spiers

Water samples for analysis were collected from a large set of lakes in Northeastern Ontario, spanning the Sudbury and Temagami areas. Metal concentration in the water samples from the lakes was measured using a combination of inductively coupled plasma emission (ICP-AES) and mass spectroscopy (ICP-MS), with anion concentration being determined by ion chromatography. Both spatial and statistical analysis was performed on the analytical results obtained for these samples. Examination of the analytical results shows that water chemistry composition follows a logarithmic distribution. The mean concentration of water chemistry parameters for most elements in acidic and circumneutral lakes was significantly different, with levels of trace elements being higher in acidic lakes and levels of Group II elements being higher in circumneutral to alkaline lakes. Regional analysis illustrated by application of mapping techniques suggest that a large regional impact zone may no longer be recognizable in the region surrounding Sudbury using content of individual elements in lake waters. The "Sudbury footprint" on the aquatic environment is less prominent indicating that cut backs in emissions have had a positive effect on the regional aquatic environments.

P18 Applications of AFS to the Monitoring of Metals in Electronics Materials

Graeme Spiers, Yan Jun, Liu Mingzhong, Chen Zhixin, Liu Jixin, He Ying, Wang Anbang

The development of legislation in Asia, Australasia, China, Europe, and North America is providing a series of strict international standards for the development and disposal of electrical and electronic products for specified chemicals of concern (COC's), specifically arsenic, cadmium, hexavalent chromium, lead, mercury and brominated flame retardants (polybrominated biphenyls and diphenyl ethers). The

international standards, generally referred to as the RoHS (Restriction on Hazardous Substances) and WEEE (Waste Electrical and Electronic Equipment), generally allow concentrations of 0.1% (or less) for all listed substances except cadmium, for which the allowable maximum is 0.01%. Atomic fluorescence spectroscopy (AFS) has been successfully utilized to quantify levels of the above legislated metals and metalloids controlled with the RoHS and WEEE legislations. This presentation will highlight the development of digestion techniques for electronic components to provide solution matrices for vapour generation methodologies for As, Cd, Cr, Hg and Pb. The application of specialized AFS instrumentation for the quantitation of elemental or hydride vapours will be highlighted.

P19 An Accurate pKa Determination of Monomeric PFOA and its Environmental Implications

Darcy Burns, Hongxia Li, Eva Webster, Lisa Reid, Don Mackay, David Ellis

The persistence, bioaccumulation potential, and possible toxicity of perfluorooctanoic acid (PFOA) has prompted increased efforts from the scientific community to better understand its long-range transport and environmental dissemination. Until now, these efforts have been directed towards the study of PFO (deprotonated PFOA) because the percentage of acid in an environmental system is thought to be negligible. However, this assumption has been based on pKa values for which PFOA is in equilibrium between an aggregated and monomeric state; a situation that is not likely to be encountered at environmental concentrations. Herein are presented two methods, a titrimetric-based method and a quantitative ^{19}F NMR-based method, which together probe the influence of aggregation on PFOA pKa. From these studies it was found that aggregation significantly lowers the pKa of PFOA, and that the measured value is in fact the equilibrium-weighted average of both the monomeric and aggregated species. The pKa of monomeric PFOA was found to be 3.4. In general, the environmental fate of PFCAs, including PFOA, has been associated with anion transport (i.e. deprotonated PFO⁻) via ocean-water flux, atmospheric decomposition of fluorotelomer alcohol (FTOH) analogues, as well as atmospheric marine aerosol transport. These models have been put forward based on the assumption that the pKa of PFOA is ~ 2.5. However, we have found that the pKa of monomeric PFOA is 3.4, so that at normal environmental pHs there will exist a significant proportion of PFOA in solution (ca. 10% in rainwater, pH 4.5). Given the K_{aw} of PFOA, large bodies of water such as lakes and oceans may now be considered as a viable source of PFOA to the atmosphere.

P20 A Mass Balance of the Distribution of Bioavailable Hg²⁺ Among Cellular Compartments of Genetically Modified *E. coli* after Exposure to Hg Solutions

Ralph Bona, Holger Hintelmann, Steven Rafferty

Mass balance experiments were conducted to determine the more relevant measure of Hg bioavailability in bacteria using two genetically engineered strains of *E. coli* (M3T and M4) i.e. whether it is total Hg taken up (internalized) from solution or only that which is found in the cytosol. M3T and M4 express the cytosolic protein metallothionein (MT) fused to glutathione sulfur transferase (GST) that could bind with Hg following uptake; the former strain also has Hg-specific (mer) transport proteins that could facilitate Hg transport across the membrane into the cytosol. The distribution of Hg within the cell following uptake depends on its initial concentration in solution. At Hg concentration of 10 ng/L, 20 and 53 % of the Hg were taken up by M4 and M3T, respectively; and up to 46 and 79 % of these reached the cytosol of the corresponding strain. But at 4×10^3 times this Hg concentration, both strains drastically reduced the amount of their internalized Hg to 3 and 13 %, respectively, whilst their cytosolic Hg remained unaffected. In fact the level of Hg in the cytosol of M3T cells increased to 86 %. And although maximum Hg uptake by these bacteria is known to occur within 10 min of exposure, a time-course experiment on Hg transfer from the periplasm to cytosol attained a maximum cytosolic Hg after 5 hr in both strains; M3T showed a peak of 95 % cytosolic Hg as against 60 % in M4. Hence, the choice of a measure of bioavailability depends on the time of exposure; uptake time may have to be extended from 10 min to 5 hr if cytosolic Hg is used, *in lieu* of internalized Hg.

P21 Luminescence Spectra of Square-planar Pt(II) Complexes at Variable Pressure and Temperature

Alexandre Rodrigue-Witchel, Christian Reber

A series of square-planar Pt(II) complexes were analyzed in a luminescence and Raman study at variable pressure and temperature. The orientations of the ligands of each of these complexes have a very big effect on the luminescence. Small changes in these ligands have an important effect on the luminescence spectra. Lowering the temperature yielded better peak resolution. Adding pressure with a diamond anvil cell to complexes had an effect on the observed luminescence. In one of the Pt(II) complexes, the addition of pressure changes the observed transition from a metal-ligand charge transfer to a ligand-centered transition. The change in transition can be analyzed as being caused by both intermolecular or intramolecular interactions. Significant shifts of the luminescence band can be observed under pressure. Red shifts between -15 and $-25 \text{ cm}^{-1}/\text{kbar}$ are recorded for band maxima from the pressure experiments. An organometallic complex was also analyzed in study.

P22 The Processes of Nickel Partitioning in the Water Column of a Recovering Lake in the Sudbury, Ontario Region

Nader Kharouba, Holger Hintelmann, Peter Dillon

Nickel (Ni) is still found at toxic levels in the water of lakes in the Sudbury area. There has been no investigation of the processes of partitioning of nickel in the water column of Clearwater and other lakes recovering from elevated metal levels and high acidity. Three commonly known factors: pH, redox potential (ORP) and organic matter (OM) concentration can influence metal partitioning in freshwater dimictic lakes. Limited knowledge on Ni fate in Sudbury waters suggested that Ni occurred mostly as free ion or labile complexes, and sediments acted as a sink for Ni (& Cu). As the lakes continue to recover, with relatively low [TOC] and [HS], the actual mechanism of partitioning and possible removal of particulate Ni is still unknown. Water column and Close interval sampling (C.I.S.) in the hypolimnion were performed in the summer of 2005 & 2006. Operationally-defined dissolved (MeD) and particulate (MeP) Ni, Cu, Co, Mn, Fe, and Al data was combined with pH, ORP, [TOC], and other parameters to provide spatial and temporal evidence for particulate Ni formation and accumulation in the hypolimnion of Clearwater Lake. We observed a benthic nepheloid layer (BNL: defined by MeP, lower pH, elevated [IC], increased alkalinity, and decreased [TOC] at the 20 & 10cm levels of the C.I.S in the main 14m basin, and at 16m to 19m in the deeper basins. This layer occurred above the sediment-water interface during peak stratification and early mixing below the thermocline, once the stratification was stable (lowest D.O. levels in the BNL & below the thermocline; and using [MeP] time series & depth profiles). Decreased [TOC] in the BNL implies the consumption of TOC during particle accumulation (inorganic/organic) or surface metal complexation onto zpc-favoured Fe-oxide colloids associated with an organic bio-film matrix. SEM-EDS backscatter scans of the collected particles support this scenario, where fine particle clusters and coarser particles (25%) are found in an organic-rich finer matrix with minor amounts of iron (75%). The SEM particles included orthorhombic sub-translucent prismatic FeO.OH (lepidocrosite) crystals and radiating growths, never observed before at this lake. EDS Spectra showed enrichments of Fe and O with minor peaks of Ni, Co, Cu, Mn, and Al in fine-grained coatings on degraded organic matter.. Since NiP was barely extractable from particle collection filters at peak stratification, it seems that Ni is removed in relatively small values through surface complexation on Fe-oxides surfaces or as co-precipitates associated with Fe-oxides and organic matter as part of an overall colloidal pumping process, confirmed by negative correlations of Ni log KD (L/kg) with log Cp (i.e. [particle]; kg/L). No Ni sulphides were observed or free sulphides detected. Future laboratory experiments testing the effects of increased sulphide concentrations, and the effect of other metals (e.g. Fe, Cu, Mn, Al, and Co) on particulate Ni formation.

P23 KINETEQL: A Sophisticated Excel Add-In Function for Computing Chemical Equilibria and Kinetics Using the Tableau Method

Robert Hudson

The tableau, or matrix, method of solving chemical equilibrium problems serves as the basis for several programs commonly used for aqueous chemical speciation calculations, such as MINEQL, MINEQL+, MINTEQA2, and Geochemists' Workbench. The method is increasingly used in aqueous geochemistry textbooks, and even some research publications, as a means of systematically organizing the mass law and mole balance equations involved in chemical equilibrium problems. An important, albeit less common, extension of the tableau method permits the systematic specification of the parameters necessary to calculate rates of chemical reactions when coupled to pseudo-equilibrium reactions, both under steady state (STEADYQL) and transient (in various reactive transport codes) conditions. KINETEQL is a Microsoft Excel Add-In function (dynamically-linked library) written in ANSI-C that uses Excel spreadsheets as the interface by which chemical equilibrium tableaux, or matrices, are entered by the user and passed to a Newton-Raphson equilibrium solver routine. The KINETEQL/Excel interface can also be used to input and solve modified tableaux used for kinetics calculations. The advantage of using Excel as the interface for the solver is that the calculations can be dynamically linked to graphs and spreadsheet models, thereby facilitating experimentation with chemical models for educational and research purposes. This poster will include a live version of the program running on a laptop and provide an opportunity to obtain the current alpha version of the software at no cost.

P24 DSC, TGA, DTA, SEM and FT-IR Spectral Studies, and Influence of 1, 10-Phenanthroline on Potassium Hydrogen Phthalate Crystals

G. Madhurambal, S. Meenakshisundaram, S. Parthiban, Subhash Mojumdar

Thiourea lead to an increase in the growth rate and improvement in the quality of different crystals. The growth promoting effect (GPE) is due to the complexation of trace metal ion impurities in solution. The resulting complex does not enter into the crystal. The influence of a new organic additive, chelating agent 1, 10-phenanthroline (Phen) ($\sim 5.0 \times 10^{-3} \text{ M L}^{-1}$) on Potassium hydrogen phthalate (KHP) ($\text{C}_8\text{H}_5\text{KO}_4$) single crystals at 30°C has been investigated. The crystals were grown from the aqueous solutions of pH ~ 4.5 at constant temperature by solvent evaporation technique. The chelating agent leads to an increase in metastable zone width and assists the bulk growth process. The growth rate of crystals in the presence of Phen decreases considerably with an increase in impurity concentration. Not much variation is observed in FT-IR and cell parameter values, determined by XRD analysis. It appears that the GPE of Phen is caused by the adsorption of the organic additive on the prism of KHP crystals. DSC, TGA and DTA studies reveal the purity of the sample and no decomposition is observed up to the melting point. SEM images exhibit the effectiveness of the impurity in changing the surface morphology of KHP crystals. Contrary to expectations, Phen depresses the NLO efficiency of KHP, suggesting that the molecular alignments in the presence of Phen results in cancellation effects disturbing the non-linearity.

P25 Thermoanalytical Characterization and Antibacterial, Antiyeast and Antifungal Activities of Mg(II) and Cu(II) Compounds with Bioactive Ligands

Mazen Saleh, Subhash Mojumdar

It is well-known that many heterocyclic compounds play an important role in many biological systems. Thermogravimetry (TG), differential thermal analysis (DTA) and spectral analysis have been used to investigate thermal behavior and structure $\text{Mg}(\text{ac})_2(\text{mpc})_{3.3}\text{H}_2\text{O}(\text{I})$, $\text{Mg}(\text{Clac})_2(\text{mpc})_{2.3}\text{H}_2\text{O}(\text{II})$, $\text{Mg}(\text{Cl}_2\text{ac})_2(\text{mpc})_{2.3}\text{H}_2\text{O}(\text{III})$, $\text{Mg}(\text{Cl}_3\text{ac})_2\cdot\text{mpc}(\text{IV})$ and $[\text{Cu}(\text{ac})_2(\text{mpc})]_{2.2}\text{H}_2\text{O}(\text{V})$ ($\text{ac} = \text{CH}_3\text{COO}^-$, $\text{Clac} = \text{ClCH}_2\text{COO}^-$, $\text{Cl}_2\text{ac} = \text{Cl}_2\text{CHCOO}^-$, $\text{Cl}_3\text{ac} = \text{Cl}_3\text{CCOO}^-$ and $\text{mpc} = \text{methyl-3-pyridyl carbamate}$). Thermal decomposition of these compounds is the multi-stage process. The possible scheme of destruction of the compounds is suggested. Heating the compounds first results in a release of water molecules. In complexes I, II and IV the loss of the volatile ligand (mpc) occurs (on the TG curves) in one step (-2mpc) and in complex III and V in two steps (-mpc, -mpc). The final products of the thermal decomposition were MgO or CuO. The thermal stability of the complexes can be ordered in the sequence: $\text{I} = \text{II} < \text{IV} < \text{III} < \text{V}$. Mpc was coordinated to Mg(II) and Cu(II) through the nitrogen atom of its heterocyclic ring. IR spectral

data suggest to a unidentate coordination of carboxylates to Mg(II) and Cu(II) in complexes I-V. The preliminary studies have showed that the compounds do have antimicrobial activities against bacteria, yeast and fungi. The highest antimicrobial activities were manifested by the compounds V on *Microsporum gypseum* (IC50 = 200 and MIC = 400 $\mu\text{g/mL}$).

P26 Characterization of ADP and KDP Crystals using TGA-DTA, FTIR, XRD, SEM and Microhardness

G. Madhurambal, S. Meenakshisundaram, S. Parthiban, R. Dhanasekaran, Subhash Mojumdar

Potassium dihydrophosphate, KDP (KH_2PO_4) and ADP ($\text{NH}_4\text{H}_2\text{PO}_4$) are widely used as the second, third and fourth harmonic generators for Nd:YAG and Nd:YLF lasers. The crystals are widely used for electro-optical applications as Q-switches for Nd:YAG, Nd:YLF, Ti:Sapphire and Alexandrite lasers, as well as for acousto-optical applications. 1,10-Phenanthroline (Phen) as a new additive was added into the solutions of ADP and KDP in a small amount ($\sim 2.5 \times 10^{-3} \text{ M L}^{-1}$). The growth rate of crystals in the presence of Phen decreases considerably with an increase in impurity concentration ($\sim 2.5 \times 10^{-2} \text{ M L}^{-1}$). Not much variation is observed in FT-IR and XRD of pure and doped ADP and KDP. It appears that the growth promoting effect (GPE) of Phen is caused by the adsorption of the organic additive on the prism faces of ADP and KDP crystals. Higher optical transmittance is observed in the presence of the dopant. Detailed microhardness studies of ADP crystals reveal the anisotropy in the hardness behaviour. SEM images exhibit the effectiveness of the impurity in changing the surface morphology of ADP and KDP crystals. Contrary to expectations, Phen depresses the NLO efficiency of ADP and KDP, suggesting that the molecular alignments in the presence of Phen results in cancellation effects disturbing the non-linearity. Simultaneous TGA-DTA studies reveal that there is no physically adsorbed water in the molecular structure of crystals grown from Phen added ADP solution. TGA curve also shows a gradual mass loss and residual mass obtained at 650 °C is only 36.13%.

P27 Thermal, Spectral and X-Ray Analysis and Fungicidal Activities of Novel Fungicides

Mazen Saleh, H. Rathore, G. Varshney, Subhash Mojumdar

There are a wide variety of compounds of anions such as dithiocarbamate, dithiocarbonate, dithiocarboxylate, trithiocarbonate, xanthate, thioxanthate, dithiophosphinate and dialkyldithiophosphinate. Each of these ions may have a corresponding monothio analogue that is S, O bound. Heavy metal dithiocarbamate and dithiophosphinate complexes are used as fungicides, solvent extractants and high pressure lubricants. They are normally made by treating the solution of heavy metal salt with sodium diethyldithiocarbamate or dimethyldithiocarbamate or dithiophosphinate or dialkyldithiophosphate. New zinc diethyldithiocarbamate, zinc diethyldithiocarbamate-phosphate and zinc phosphate have been prepared by treating aqueous zinc sulphate solution with sodium diethyldithiocarbamate and trisodium phosphate. These compounds have been characterized using DTA-TGA, IR, X-ray and volumetric analyses. DTA and TGA of zinc diethyldithiocarbamate show only one peak and one main plateau at 330 °C (weight loss = 83.18 %). The results of DTA and TGA for zinc diethyldithiocarbamate-phosphate under study were found to be almost similar to that of zinc diethyldithiocarbamate. Thus the procedure used yields zinc diethyldithiocarbamate, which contains zinc phosphate as impurities at traces. In case of zinc phosphate four peaks are obtained at 92 °C (weight loss = 7.6 %), 115 °C (weight loss = 22.33 %), 286 °C (weight loss = 1.81 %) and at 330 °C (weight loss = 4.16 %). Fungicidal activity along with results obtained by IR spectra, X-ray, spectrophotometric and volumetric analyses are also discussed in this paper.

ABSTRACTS – MC WORKSHOP

Application of MC-ICP-MS to Nuclear Problematics

Anthony Nonell, Frédéric Chartier, H  l  ne Isnard

In nuclear industry, the knowledge of elemental and isotopic compositions of fission products and actinides is crucial for qualification of neutronic calculation codes and management of nuclear wastes. TIMS and MC-ICP-MS facilities, available at the Laboratory of Nuclear, Isotopic and Elementary Analyses (French Nuclear Agency, Saclay, France) are used to investigate on these purposes. One of the major objectives in this research area is to obtain absolute isotopic compositions with high accuracy and precision. In nuclear samples, most of the isotopes of interest are affected by radioactive decay and isotopic abundances are generally very different from those observed in natural samples. As a consequence, conventional corrections for instrumental mass bias, widely used in geosciences, such as internal normalization to an invariant ratio, are generally not suitable for nuclear applications. Therefore, different analytical strategies are used to obtain the highest accuracy and precision on the isotopic compositions of nuclear samples. By using recent MC-ICP-MS developments on the isotopic analyses of rare earth elements in nuclear fuel samples, both similarities and differences between nuclear strategies and the various approaches used in geosciences for the determination of isotopic compositions will be illustrated. In addition, possible applications of collision/reaction cells for direct separation of isobaric interference in nuclear samples analyses will be presented.

Mass-independent Variation in the Stable Isotope Composition of Mercury in Methylmercury Accumulated by Freshwater Food Web Organisms

Togwell Jackson, Michael Whittle, Marlene Evans, Derek Muir

Variations in the stable isotope composition of mercury (Hg) in the environment could provide valuable information on the sources and biogeochemical cycling of the Hg; yet little is known about the subject, and until the advent of multicollector inductively coupled plasma mass spectrometry (MC-ICP-MS) it posed formidable technical difficulties and was rarely investigated. Using MC-ICP-MS (performed by Activation Laboratories Ltd.), we determined the stable isotope composition of Hg in crustaceans, fish, and sediment cores from Lake Ontario and two remote boreal forest lakes. Standard and sample solutions were analyzed in the order standard-sample-standard, and their $^{198}\text{Hg}/^{202}\text{Hg}$, $^{199}\text{Hg}/^{202}\text{Hg}$, $^{200}\text{Hg}/^{202}\text{Hg}$, and $^{201}\text{Hg}/^{202}\text{Hg}$ ratios were used to calculate corresponding α -values. Total Hg, methylmercury (MeHg), and C and N isotope analyses were done as well. Our purpose was to investigate fractionation of Hg isotopes in freshwater ecosystems. Evidence for mass-independent fractionation of Hg isotopes, with selective enrichment in isotopes with odd mass numbers (^{199}Hg and ^{201}Hg), was found in all biological samples, but only mass-dependent variation occurred in sediments. The mass-independent isotope effect increased with MeHg concentration, and hence with trophic level (though lake whitefish gave aberrant results consistent with biochemical demethylation). Isotope signatures also varied with habitat and diet. Analysis of MeHg and inorganic Hg extracts from fish proved that the mass-independent isotope effect was due to anomalously high abundances of ^{199}Hg and ^{201}Hg in MeHg accumulated by the organisms, as implied by the data for whole organisms, suggesting that microbial methylation of Hg causes mass-independent fractionation of Hg isotopes. The phenomenon is attributable to effects of nuclear spin or field shift, or both, and penetration of the inner electron shells of Hg by valence electrons of ligands owing to the high nuclear charge of Hg and weak shielding of it by d- and f-electrons.

MC-ICP-MS-The Nightmare of Matrix, Mass Bias and Mass Fractionation

Don Chipley, Kurt Kyser

Initially, it was thought that isotope ratios could be measured by MC-ICP-MS with minimal sample preparation, just dissolve and dilute. However, as we have gained experience in isotopic analysis using this technique, for most elements this does not hold. Low mass elements in particular exhibit significant mass fractionations, such as Li with 25 to 30 % mass fractionation, and require separation of the element

from matrix. Furthermore, the concentrations of the elements in the samples must be matched to the concentration of the isotopic standard to measure correct isotope ratios. Slightly heavier elements with masses greater than Sr or elements that behave as anions, such as S, can be measured accurately in low TDS matrices, but again it is necessary to match the sample and standard concentrations. Strontium isotope ratios can be measured in solutions with higher TDS, such as carbonates, but for high precision measurements, $1s < 0.00001$, separation is still a necessity. Additionally, measurements of the strontium isotopic standard, NIST 987, with variable amounts of Rb added, reveals that the ^{87}Rb cannot be correctly subtracted from ^{87}Sr using $^{88}\text{Sr}/^{86}\text{Sr}$ to account for the mass fractionation effects on Rb. This suggests that there is an influence on the isotope responses that is not completely mass dependant and that high precision measurements are not yet achievable in samples that contain Rb. Lead isotope ratios are a very useful means for distinguishing a variety of anthropogenic sources. Further, uranium and lead have been found to behave well when measured either by laser ablation or in solution. Ages using the U-Pb system can be extracted from minerals with acceptable accuracy and precision. Much of the variability in U/Pb and Pb/Pb isotope ratios measured by laser ablation of natural samples can be attributed to variable resetting of the U-Pb systematics in the mineral rather than effects from the MC-ICP-MS.

MC-ICP-MS faults, cures and other fishy tales

Peter Stow

As modern instruments have evolved the interface with the instrument has become more reliant on computer technology. In this new world how can operators who cut their teeth on "knobs, dials and meters" discover what ails their instrument.

Determination of Isotope Ratios from Transient Signals evolved from MC-ICP-MS Measurements

Mark Dzurko, Delphine Foucher, Holger Hintelmann

Due to the commercial introduction of Multi-Collector Inductively Coupled Plasma-Mass Spectrometry (MC-ICP-MS), new isotope systems are being studied that deviate from traditional geochemical applications. Measurements of natural fractionation of non-traditional isotopes are a powerful tool to directly identify biogeochemical processes controlling the fate of these elements in the environment, yet research is demonstrating that the chemical species of these elements are important in the various physical and chemical processes, so tracing species-specific isotope ratios necessitates the proper elucidation of isotope ratios from transient signals. Several methods for isotope ratio determination will be presented and evaluated for their precision and accuracy from the transient signals. Discussion will revolve around whether these measurements are realistic, is this where the future MC-ICP-MS research is going?, can we expect larger fractionation when looking at species individually?

Selective Separation of Selenium (IV) by Cellulose Thioglycolic Acid Powder

Nagmeddin Elwaer, Holger Hintelmann

A simple and efficient matrix separation procedure for the removal of hydride-forming elements such as As, Ge and Sb and transition metal ion interferences is described for the determination of selenium (IV) by hydride generation SF-ICP/MS. The uptake of Se ions by cellulose thioglycolic acid (CTG) derivatized cellulose powder was studied by both batch and column methods. The selective separation of Se (IV) from the interferences was achieved with a column method using 0.10g of CTG powder and eluting the interfering species with dilute hydrochloric acid prior to analysis. The procedure was also used for pre-concentrating Se from several liters of lake water. The degree of pre-concentration was linearly proportional to the amount of sample passed through the column. Se retained on the CTG powder was quantitatively recovered by digesting twice with a small volumes (50 μl) of concentrated nitric acid. The method was initially applied to determine Se concentrations in lake sediments and certified reference materials. Good agreement was obtained between the certified values and the experimental results. The complete elimination of interfering elements and the marked gain in sensitivity makes this method particularly useful as a sample preparation scheme for subsequent high precision Se isotope ratio measurements using techniques such as multicollector ICP/MS.

Fe Isotopic Analysis by MC-ICP-MS in Nutritional Studies: Beyond the Challenges

Karima Benkhedda, Kevin Cockell

Stable isotopes provide a safer alternative to radiotracers for studying mineral nutrient metabolism in humans. Iron (Fe) is an essential mineral whose bioavailability has been extensively assessed in nutritional studies. This led to strategies aiming at decreasing the prevalence of Fe deficiency in both developed and developing countries. Multicollector-ICP-MS constitutes the latest innovation in producing high precision isotopic ratio measurements, compared to other mass spectrometers based on a single collector. However, several potential limitations complicate Fe isotopic analysis and still need to be addressed, such as spectral (molecular and or isobaric) interferences on all four isotopes and non-spectral (from the sample matrix) interferences. In addition, adequate sensitivity is required for achieving accurate isotopic ratios involving Fe isotopes with a lower abundance such as ^{58}Fe . Therefore one or a combination of strategies is necessary to permit the determination of at least 3 isotopes to be applied in dual tracer studies. After sample decomposition, analyte separation from sample matrix, aerosol desolvation, mass bias correction, mathematical corrections for the unresolved isobaric interferences, blank and background subtraction, is it still realistic to aim at achieving the adequate and necessary precision and accuracy to obtain meaningful isotopic enrichment after isotope administration? We outline our own experiences with the measurement of Fe isotopic ratios by a VG-Axiom-ICP-MS to be applied in a study examining Fe absorption in women receiving calcium supplements.

Potential Interferences in MC-ICP-MS and Impacts on High Precision Isotope Measurements: Using B as an Example

Qianli Xie, Peter Dillon

In high precision isotope analysis, it is a common practice that one uses ion chromatography to separate analyte of interests from other matrices, and hence minimize potential isobaric and polyatomic species interferences, for examples in high precision stable isotope analysis of Fe, Cu, Zn, Sr, Nd, Pb etc. There are, however, potential interferences deriving from sample matrices that can not readily be avoided, such as polyatomic species from solution matrices (e.g. HNO_3 and H_2O), Ar and impurity in gases. These interferences may not be easily detectable, and are not readily attributable to the sources, unless one uses higher resolution power. In this regard, an MC-ICP-MS with higher resolution power will certainly be advantageous. In this discussion, we will use B isotope measurement as an example to illustrate the potential interference and its impact on the precision and accuracy.

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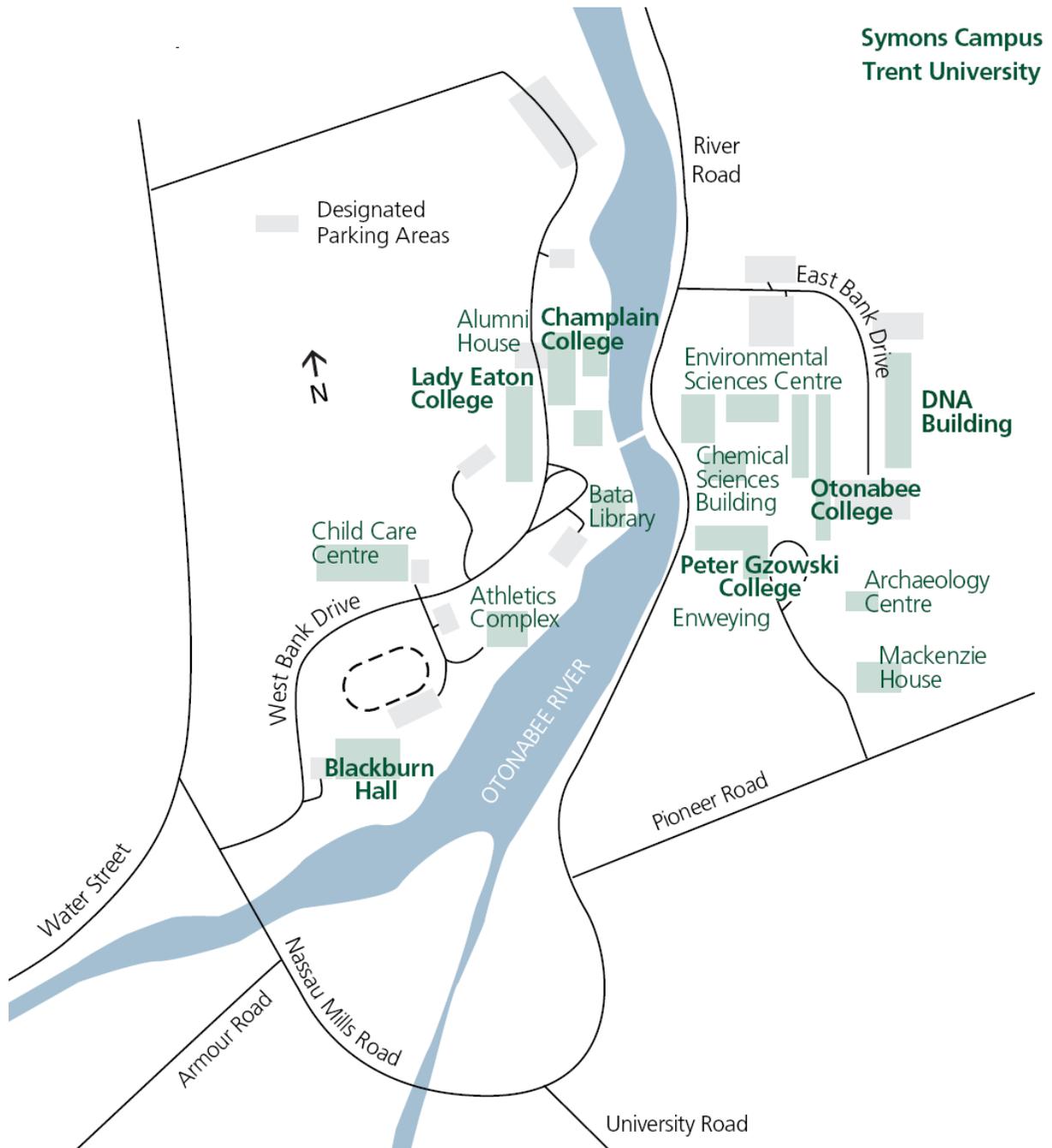
INDEX OF PARTICIPANTS – MC WORKSHOP

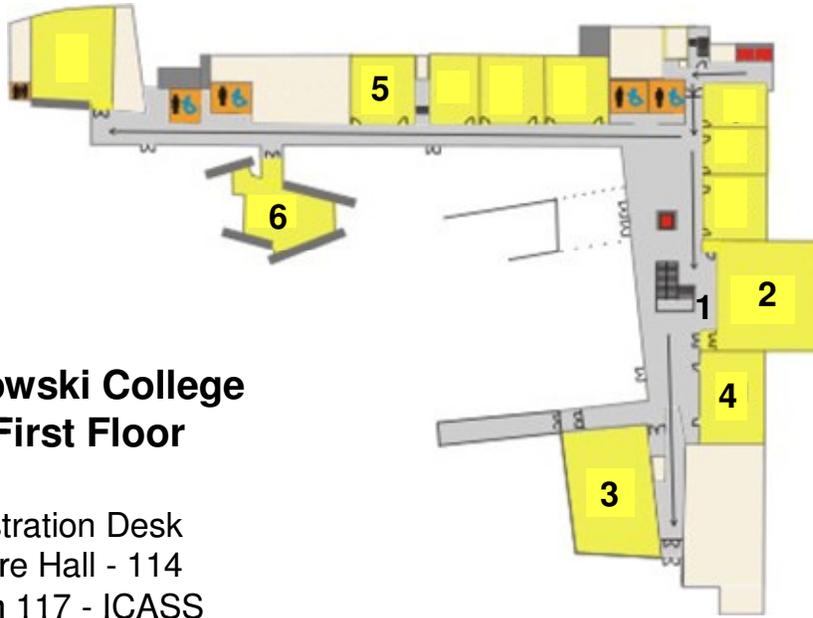
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MAPS

Trent University - Campus Map



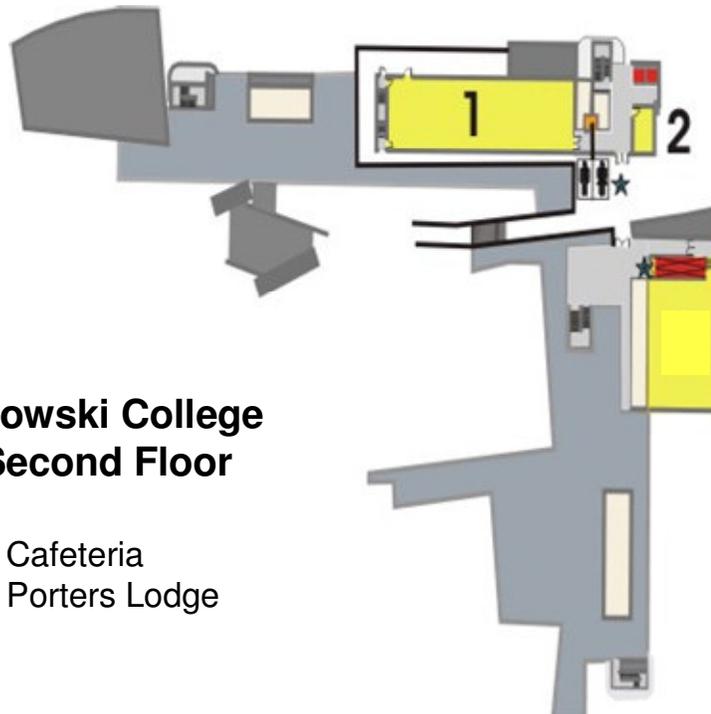


**Gzowski College
First Floor**

- 1 Registration Desk
- 2 Lecture Hall - 114
- 3 Room 117 - ICASS
- 4 Room 115 - CTAS
- 5 Speaker Ready Room - 103
- 6 Exhibitors Hall - 102

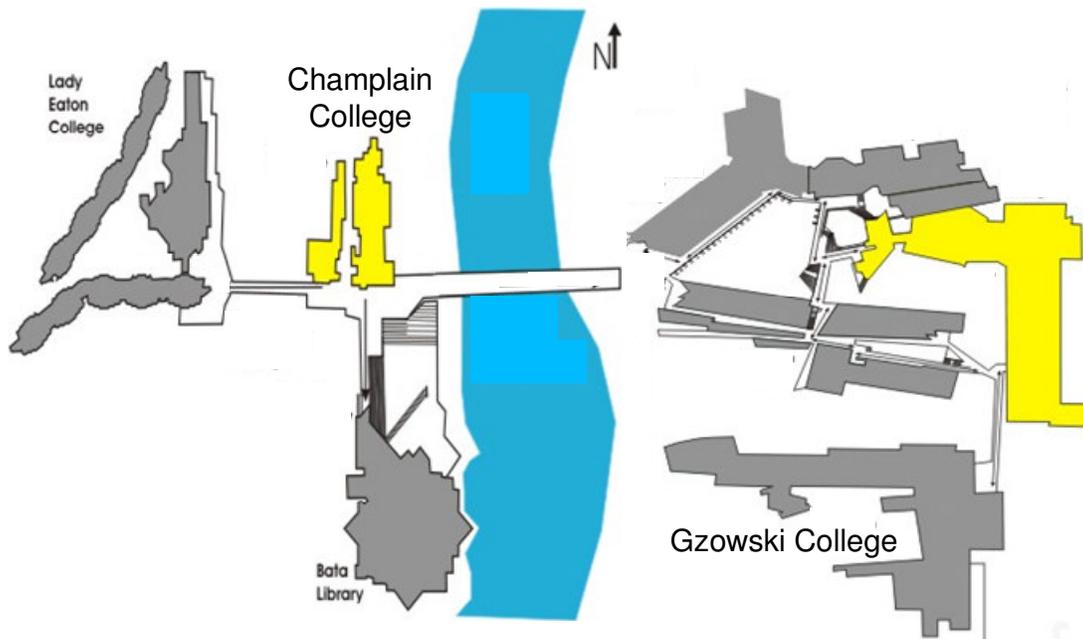
Legend

Accessible Rooms	Automatic Door Openers
Non-Accessible Rooms	Ramp
Partial Accessible	Hearing Adaptive Rooms
Faculty Offices and Labs	Elevator
Washrooms	Refuge Area



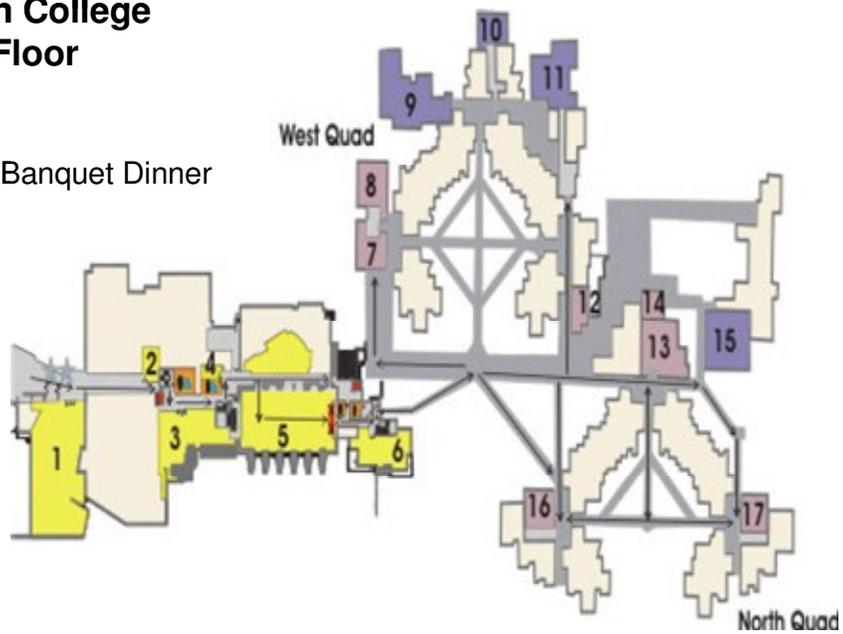
**Gzowski College
Second Floor**

- 1 Cafeteria
- 2 Porters Lodge



**Champlain College
First Floor**

- 1 Bookstore
- 5 Great Hall – Banquet Dinner



PETERBOROUGH DIRECTORY

Your organizers' pick:

Brio Gusto

182 Charlotte St.
Phone: 745-6100
Style: Fine Dining

Cosmic Charlie's Café

170 Charlotte St.
Phone: 741-6491
Style: East Asian Cuisine

Curry Village

306 George St. S.
Phone: 742-1432
Style: Indian Cuisine

Hot Belly Mama's

378 George St. N.
Phone: 745-3544
Style: Cajun-Creole

Karma's Café

217 Hunter St. W.
Phone: 748-5451
Style: Himalayan Cuisine

38 Degrees

375 Water St.
Phone: 750-0038
Style: Fine Dining

Matsu Korean & Japanese Restaurant

733 Park Street S.
Phone: 876-7765
Style: Japanese and Korean Cuisine

Night Kitchen Pizza

222 Hunter St. W.
Phone: 741-0300
Style: Specialty Pizza Shop

Olde Stone Brewing Company

380 George St. N.
Phone: 750-0495
Style: Brew Pub

St. Veronus Café & tap Bar

129 Hunter St. W.
Phone: 743-5714
Style: Belgian Cuisine

