CENTRE FOR RESEARCH IN MASS SPECTROMETRY (CRMS)

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Background and Mandate

In April 2000, the University's Senate endorsed the creation of an organized research unit specializing in mass spectrometry research. The unit, known as the Centre for Research in Mass Spectrometry (CRMS), draws upon faculty from Chemistry and Biology, and MDS Analytical Technologies (AT, formerly SCIEX). The aim of the centre is to promote and actively seek interdisciplinary and collaborative research in mass spectrometry, and highlight the importance of mass spectrometry as a discipline.

Executive Committee

D.K. Bohme
A.C. Hopkinson
R.R. Hudgins
K.W.M. Siu

Organizational Structure and Staffing

Director:	K.W. Michael Siu
Administrative Contact:	Nicole Chevannes-McGregor
Seminar Coordinator:	Greg Koyanagi

Faculty Members of the Centre (2005-2008)

Vladimir I. Baranov, Adjunct Professor of Chemistry; Senior Research Scientist, MDS AT; Associate Professor, University of Toronto

Diethard K. Bohme, Distinguished Research Professor (Chemistry); Canada Research Chair (Tier I) in Physical Chemistry (Chemical Mass Spectrometry)

René Fournier, Associate Professor of Chemistry

John M. Goodings, Professor Emeritus of Chemistry

Donald R. Hastie, Professor and Chair of Chemistry

Alan C. Hopkinson, Professor of Chemistry

Robert R. Hudgins, Assistant Professor of Chemistry

John C. McDermott, Associate Professor of Biology

Ronald E. Pearlman, University Professor; Director, Core Molecular Biology Facility; Dean, Faculty of Graduate Studies

Jochen Rudolph, Professor of Chemistry

K.W. Michael Siu, Distinguished Research Professor (Chemistry); NSERC / MDS AT Industrial Research Chair in Analytical Mass Spectrometry; Director, CRMS; Associate Vice-President Research, Science & Technology

Bruce A. Thomson, Adjunct Professor of Chemistry; Principal Research Scientist, MDS AT

Derek Wilson, Assistant Professor of Chemistry

Seminars and Conferences

The CRMS runs a bi-weekly seminar series with lectures presented by students and postdoctoral fellows (PDFs) from the Centre as well as by faculty members from York University and other academic and research institutions. These lectures are more formal than the intra-group presentations that students and PDFs give, are popular, and serve as a training ground for formal presentations and have stimulated collaborations among the students and PDFs. Invited speakers from the 2007-2008 lecture series included **Prof. Gerold Schmitt-Ulms** – University of Toronto, **Prof. Chris Le** – University of Alberta, **Prof. Rob Dunbar** – Case Western Reserve University, **Dr. Julia Laskin** – Pacific Northwest National Laboratory, **Guerman Pasmanik** – Passat Ltd. and **Jim Kepka** – MesoScale Discovery

Several faculty and student members of the CRMS attended and presented their research findings at the 20th Annual Tandem Mass Spectrometry Workshop, November 28 – December 1, 2007, at Chateau Lake Louise, Alberta; and at the 56th American Society for Mass Spectrometry Conference, June 1 - 5, 2008, at the Colorado Convention Center, Denver, Colorado. The CRMS was also represented at the Human Proteome Organization's 7th Annual World Congress in Amsterdam from Aug 16-20, 2008

CRMS constituted the largest participating group at the 25th Trent Conference on Mass Spectrometry, July 28th – 31st, held at the YMCA, Geneva Park, Orillia, Ontario, with 9 oral and 6 poster presentations.

Activities

The research projects of a number of students and PDFs are conducted in collaboration with industries (e.g. MDS AT), hospitals, and hospital research institutes (e.g. Mount Sinai, St. Michael's and the Hospital for Sick Children). The interactions offer these trainees experience in larger-scale projects that integrate a number of disciplines and serve as excellent training ground for these prospective highly trained personnel of Canada.

CRMS has had a busy year. Some of the highlights are as follows:

Kudos

Daryl G.S. Smith won a CSMS Travel Award to present his work at the 20th Annual Tandem Mass Spectrometry Workshop at Lake Louise. **Janna Anichina** and **Chi-Yuet (X'avia) Chan** have won travel awards to present their work at the 21st Annual Tandem Mass Spectrometry Workshop, December 3 – 6, 2008. Congratulations!

Daryl G.S. Smith successfully defended his Ph.D. dissertation entitled "Mass Spectrometry-Based Proteomics: Qualitative and Quantitative Studies" in July 2008. He has accepted a short-term postdoctoral position at Carleton University with **Prof. Jeffrey C. Smith**, a CRMS alumnus.

Congratulations! To Dr. Smith on his new addition to his family Miss. Norah Joy Smith, born on August 14, 2008.

Michael Jarvis received the Susan Mann Dissertation Scholarship from York University for his final year as a Ph.D. student with Dr. Bohme.

Daryl Smith, a Ph.D. student of Dr. Siu, won a Canadian Society for Mass Spectrometry Travel Award to present his research findings at the 20th (2007) Lake Lousie Tandem Mass Spectrometry Workshop; Daryl also won a travel award to attend the National Cancer Institute of Canada's 60th anniversary conference and public forum.

Diethard Bohme was awarded the CIC Medal for his significant and sustained contributions to chemistry from the Chemical Institute of Canada in June 2007. The CIC Medal is the highest honour awarded by the Institute.

K.W. Michael Siu received the 2007 New Pioneers Award in Science and Technology from Skills for Change for his significant contributions as a (former) immigrant and a Distinguished Research Professorship from York University in June 2007.

Graduations Training Activities/Accomplishments.

Daryl Smith, a Ph.D. student under the supervision of Dr. K.W. Michael Siu, received his dissertation entitled "Mass spectrometry-based proteomics: qualitative and quantitative studies".

Tujin Shi, a Ph.D. student under the co-supervison of Drs. Hopkinson and Siu, received his Ph.D. degree for his dissertation entitled "Fragmentation Chemistries of Multiply Charged Metal Ions Associated with Small Organic Compounds and Peptides: Theoretical Examination and Experimental Study". Dr. Shi is now a postdoctoral fellow at the Centre for Research in Neurodegenerative Diseases, University of Toronto.

Sara Hashemi, a Chemistry graduate student of Dr. Bohme, received a M.Sc. degree for her thesis on "ESI/MS Studies of Fragmentation of Metallated Phthalocyanines".

Svitlana Prada, a Physics and Astronomy graduate student co-supervised by Drs. Baranov and Bohme, received her Ph.D. degree with a dissertation on "Comprehensive Mass Spectrometric Analysis of Novel Organic Semiconductor Molecules".

Leroi V. DeSouza, a Ph.D. student of Dr. Siu, successfully defended his Ph.D. dissertation on "Cancer Biomarker Discovery Using Mass Spectrometry". Dr. DeSouza continues as the Proteomics Facility Manager and Senior Project Scientist with Dr. Siu.

Yuzhu Guo, a Ph.D. student of Dr. Siu, received her Ph.D. degree for her dissertation on "Investigation of Gas-Phase Ion Conformation by Ion Mobility Spectrometry". Dr. Guo is now a postdoctoral fellow at CRMS spearheading collaborative research work between Drs. Thomson and Siu.

Dr. Bohme's research continues to focus on the investigation of metallic, organometallic and biometallic ion chemistry and has now expanded further into biological ions and ion chemistry. An inductively coupled plasma / selected-ion flow tube / triple quadrupole (ICP/SIFT/QqQ) mass spectrometer has been used to study bare metal-ion chemistry and two electrospray ionization (ESI)/triple quadrupole mass spectrometers are providing information on the breakdown of selected organometallic, biological and biometallic ions. Also, an ESI/q/SIFT/QqQ configuration has been developed to study reactions of small molecules with biological and biometallic ions, including positive and negative ions of penicillins, siderophores, porphorins, phthalocyanines and oligonucleotides. Further strides have been made in characterizing periodic trends in the reactivities of bare atomic metal and lanthanide cations towards a variety of small molecules (the data are available on our web site). Early measurements with the ESI/q/SIFT/QqQ have focussed on the protonation of highly-charged anions of a 6-mer oligonucleotide and the ozonolysis of metallated peptides, porphyrin and phthalocyanine. These measurements, along with others involving ligation of metals with small segments of biological molecules, show promise for mimicking of *in vivo* biological interactions and measuring their intrinsic reactivities in the gas phase.

In 2007/08, 22 refereed papers were published by the Bohme group or are in press. Talks were again presented by student members of the group at this year's Ontario Ion Chemistry meeting in Orillia. Laura Banu presented a talk on "Gas-phase activation of amino acids by lead dications" at the 56th ASMS Conference on Mass Spectrometry in Denver. Koyanagi and Bohme presented an overview of their research to Sionex in Boston. Bohme presented an invited lecture at the CIC Conference in Edmonton in May in a symposium on Biological Mass Spectrometry entitled "From Chemical to Biological Mass Spectrometry: Active Nitrogen to DNA.

Dr. Fournier studies the geometric structure of clusters by theoretical methods. The energy is calculated by density functional theory (DFT) and is minimized by a new algorithm called the "Tabu Search in Descriptor Space" (TSDS) developed by the Fournier group. Clusters and molecular ions often have unusual structures that do not obey the simple rules of chemistry textbooks. The current TSDS algorithm systematically searches all kinds of cluster

structures, without *a priori* knowledge or assumptions, so it is able to find unusual structures. A student, Min Zhang, is developing a semi-empirical method to calculate, at a small computing cost (seconds or minutes), atomic charges, ionization energies, and electrostatic potentials. This method can treat neutral or charged systems containing up to thousands of atoms with accuracy nearly as good as DFT.

Dr. Hastie is interested in mass spectrometric analysis of atmospheric particulate matter. There is a robust connection between atmospheric particulate matter and adverse health impacts. As part of the efforts in understanding the production and fate of particulate matter, the Hastie group addresses the chemical identification of the species present in the secondary particulate matter produced from the atmospheric oxidation of gas phase hydrocarbons. This material is known to be a significant contributor to atmospheric particulate mass, but its toxicity cannot be properly studied until a more complete chemical identification is done. The ultimate aim of this work is to actually determine the chemical species produced in these oxidation reactions and those that end up in the particle phase. The identification of these compounds will permit identification of the source of particulate matter, both in terms of the precursor compounds and the sector responsible for their production. The methodology involves producing atmospherically relevant particulate matter in the laboratory from the controlled oxidation of gas phase hydrocarbons, and analyzing the products using mass spectrometry.

Dr. Hopkinson's research is in the area of application of computational chemistry to the calculation of ion structures and energetics. The bulk of his research has been carried out in collaboration with Professors Bohme and Siu. These calculations are crucial to mass spectrometry research as they provide plausible structures and energetics of experimentally measured ions and transition states involved in fragmentation pathways. These allow fragmentation mechanisms to be proposed and ion chemistry rationalized. Ions that have been examined range from dipositive and tripositive metal-centered ions, protonated and metalated oligopeptides, polysodiated ions, and peptide radical cations. Another area of computation (in collaboration with Professor Michael G. Organ, Department of Chemistry) involves the synthesis of compounds containing C-C single bonds from alkyl halides and organometalic halides using palladium complexes as catalysts.

Dr. Hudgins is currently studying the gas-phase structure and reactivity of RNA and DNA oligonucleotides. The multiple charges on an electrosprayed, gas-phase oligonucleotide are found to greatly affect the gas-phase oligonucleotide conformation. This result suggests that designed chemical modifications are necessary, by which charges can be arranged in the oligonucleotide. An optimum arrangement of the multiple charges would minimize the perturbation of oligonucleotide solution-phase structure that occurs upon transfer to the gas phase. By minimizing the effect of the charges in the gas phase, gas-phase conformations relevant to the solution-phase conformations (in solution, the aqueous solvent screens the ion charges) may be observed. In this way, mass spectrometry can be used more effectively to study biologically relevant oligonucleotide conformations, in the gas phase. These charge-sequestering oligonucleotide modifications will be pursued in the coming years. Ideally, the reactivity of native-like oligonucleotide structures in the gas phase can then be examined. Reactivity studies will focus on intercalating drugs, e.g., those that bind within the grooves of double-stranded DNA.

Dr. McDermott's mass spectrometry-related research centers on the phosphorylation status of an important protein, myocyte enhancer factor (MEF) 2A, which is a member of a family of transcriptional regulators recognized for heart and skeletal muscle development and in the protection of neuronal cells from apotosis. In the last year, several novel phosphorylation sites on MEF2A were identified, and significant advancement in the understanding of MEF2A regulation was also made. These constitute the basis of a collaboration with Stratagene, La Jolla, CA, on the development of tandem affinity purification for producing significant quantities of proteins for mass spectrometry characterization.

Dr. Pearlman's mass spectrometry-related research has continued to focus on the development of proteomics approaches with the model eukaryotic microorganism, the ciliated protozoan *Tetrahymena thermophila*. This work has been carried out in collaboration with Dr. Siu. A major emphasis of these studies has been on mapping of organellar proteomes using multidimensional LC/MS/MS analysis of isolated and purified organelles. This has been enabled by the availability of the complete genome sequence and a set of approximately 24,000 preliminary gene predictions (PGPs) available through public databases for three years and published in September 2006. Pearlman has been involved in leadership of the *Tetrahymena* Genome Project since its inception and is a co-author of the genome paper publication. Proteomic analysis of cilia was completed and published in 2005. The results of the analysis of the

phagosome proteome, in collaboration with Dr. Lawrence Klobutcher, University of Connecticut Health Sciences Center, were published in 2006. Examination of the mitochondrial proteome has been completed, in collaboration with Dr. Michael W. Gray, Dalhousie University. This work was published in fall 2007. This very detailed analysis provides important comparative information as essentially no data on the complete mitochondrial proteome of any protist exist. These efforts have resulted in identification of hundreds of proteins in cilia, phagosomes and mitochondria. In addition, a proteomic approach to the analysis of regulated secretion in *Tetrahymena* has also been completed and published in 2005, in collaboration with Dr. Aaron Turkewitz, University of Chicago. Additional bioinformatic analysis of cilia proteins with particular focus on homologues to human disease genes as well as *in situ* localization and functional analysis of some cilia proteins is nearing completion. An analysis of nuclear proteins in the context of function in developmentally programmed genome reorganization, some of this work in collaboration with Dr. Martin Gorovsky, University of Rochester, has been initiated and a manuscript on functional analysis of a protein identified by mass spectrometry that interacts with the small RNA-binding protein Twi1p in the process of developmental genome rearrangement and RNA-mediated irreversible gene silencing has been submitted for publication. Global analysis of the proteomes of somatic, germinal, and developing nuclei have been initiated, the work on germinal nuclei in collaboration with Dr. Emily Wiley, Claremont Colleges, Claremont, California. An NSERC Special Strategic Project Grant application with a proteomics component to use *Tetrahymena* in monitoring environmental pollutants, in particular nanoparticles, has been submitted. This project is a collaboration with Dr. Siu and with Dr. Eduardo Orias, University of California, Santa Barbara.

Dr. Rudolph is interested in characterization of secondary organic aerosols (SOAs), in particular the use of stable carbon isotope ratios in identifying their origin. Measurement of the isotope ratio of SOA formed by the photochemical oxidation of toluene in a flow reactor showed a significant fractionation between toluene and the formed secondary particulate organic matter. The observed isotope fractionation is consistent with a fractionation solely due to the kinetic isotope effect for the reaction of toluene with the OH-radical. Independent of the origin of the isotope fractionation between precursor and SOA, the results strongly suggest that the isotope ratio of the SOA depends on the degree of processing of the gas-phase precursor. It can therefore be expected that measurement of the stable carbon isotope ratio of ambient SOA will allow differentiation between recently formed and old SOA. This can be used to differentiate between SOA formed locally and SOA from long range transport. Isoprene is one of the most important organic compounds in the atmosphere and a main contributor to photochemical air pollution. Although atmospheric isoprene is predominantly due to emissions from vegetation, understanding the role of isoprene is essential for the development of effective pollution control strategies. Combining concentration with isotope ratio measurements is a very powerful tool to determine study the sources and chemistry of isoprene in the atmosphere.

Stable Carbon Isotope Ratio Studies of the Atmospheric Chemistry of Volatile Organic Compounds (VOC) -

The aim of this research is to create and expand the general data basis and concepts necessary for the application of isotope ratio measurements to study the Atmospheric Chemistry of VOC.

- Development and application of experimental methods to determine isotope ratios of VOC and VOC reaction products, including secondary particulate organic matter, in the atmosphere.
- Measurements of the kinetic isotope effects (KIEs) for reactions of atmospheric relevance including studies of the isotope fractionation during the formation of secondary organic pollutants.
- Development of conceptual and numerical tools to establish the relation between ambient measurements of stable carbon isotope ratios of organic compounds and the key atmospheric processes determining their atmospheric concentrations.

The experimental studies are based on mass spectrometric stable carbon isotope ratio measurements (IRMS) in combination with gas chromatographic separations and online conversion of the VOC to carbon dioxide or hydrogen (GC-IRMS).

These studies are conducted in cooperation with Environment Canada and the Research Center Julich (Germany).

Conferences and Presentations: R. Iannone, S. Moukhtar, R. Koppmann and J. Rudolph, 2008, Stable carbon kinetic isotope effects of the reactions of isoprene, methacrolein and methyl vinyl ketone with ozone in the gas phase, Geophysical Research Abstracts, Vol. 10, EGU2008-A-00000, 2008, EGU General Assembly, April, 2008. PDF; R. Iannone, S. Moukhtar, R. Koppmann and J. Rudolph, 2008, Stable carbon isotope ratios, mixing ratios and average photochemical ages of several light VOCs including isoprene, benzene, and toluene during May-August, 2005, measured near Juelich, Germany, Geophysical Research Abstracts, Vol. 10, EGU2008-A-00000, 2008, EGU General Assembly, April, 2008. PDF; S. Moukhtar, A. Klimkina, S. Irei, L. Huang, J. Rudolph, 2008, Study of secondary particulate matter in the atmosphere via stable carbon isotope measurements, Geophysical Research Abstracts, Vol.

10, EGU2008-A-00000, 2008, EGU General Assembly, April, 2008. PDF; Satoshi Irei, Lin Huang, Janeen Auld, Fabrice Collin, Wendy Zhang, Donald Hastie, and Jochen Rudolph, Laboratory studies of stable carbon isotopic composition of secondary particulate organic matter formed by toluene-OH radical induced reactions, Poster presented at the Annual Meeting of the Japanese Atmospheric Chemistry Organization, Nov. 26-29, 2007. POSTER

Dr. Siu's group continues to tackle a variety of subjects ranging from the very fundamental to the very applied. A series of studies have been carried out to examine the fragmentation chemistries and mechanisms of protonated peptides; fragmentation of protonated peptides constitutes the backbone in protein sequencing and identification in proteomics. Much progress has been made in exploring and understanding the structure and dissociation mechanisms of molecular radical cations of peptides, after an unprecedented method for producing these fascinating species were discovered by the Siu group in 2000. Binding chemistries of peptides to metal ions have also been examined in detail. These investigations were carried out experimentally and theoretically in collaboration with Professor Hopkinson. Much inroad has been made in building and applying new mass spectrometric hardware for innovative studies. These were carried out in collaboration with MDS AT scientists. A number of collaborative proteomic projects with biologists and biomedical scientists have resulted in significant findings. In collaboration with Dr. Terence J. Colgan, Mount Sinai Hospital, and Dr. Alexander D. Romaschin, St. Michael's Hospital, a total of 15 potential protein markers for endometrial cancer have been discovered and identified; some of these have been independently verified using immunohistochemistry and tissue microarrays. The effort in elucidating cancer biomarkers has been further augmented by collaborations on Brain cancer and Head and Neck cancer marker discovery with Dr Abhijit Guha, Hospital for Sick Children in Toronto and Dr. Ranju Ralhan from the All India Institute for Medical Sciences, New Delhi. In 2006/07, 28 refereed papers and book chapters have been published or are in press; 38 presentations were given by Siu and his group. 30 of the presentations were invited, including presentations at academic institutions (Beijing Proteome Research Center; Queen's University, University of Hong Kong, Prince of Wales Hospital, Department of Medicine and Therapeutics, Chinese University of Hong Kong, University of Toronto, Northeastern Ontario Regional Cancer Centre, Sudbury Regional Hospital, Dalhousie University, Josephine Nefkens Institute Oncology and Hong Kong Polytechnic University; conferences and symposia (4th Uppsala International Conference, Indo-Canadian Meeting on Health Biotechnology; 5th Chinese HUPO Annual Congress; Annual Symposium of Hong Kong Proteomics Society; CSI XXXV Pre-conference Symposium on New Proteomics Technology, Shanghai; Biomarker Workshop on Early Cancer Detection; Global Innovation and Commercialization through Partnerships; 20th Lake Louise Workshop on Tandem Mass Spectrometry; HUPO 5th Annual World Congress; 55th American Society for Mass Spectrometry Conference; A Canadian Cancer Research Conference Celebrating NCIC's 60th Anniversary and 20th Lake Louise Workshop on Tandem Mass Spectrometry.

Dr. Thomson's is centered on developing new tools to combine with mass spectrometry for the improved analysis of biomolecules. Work has continued on interfacing an infrared laser to a QqTOF for improved fragmentation and desolvation. IRMPD has previously been shown to be able to fragment proteins, and now has been shown to fragment large protein complexes. Additionally, there is recent evidence to show that IRMPD can help to decluster protein complexes, which should improve the ability to obtain more accurate molecular weight information. Studies of the utility of using IRMPD to fragment and decluster protein complexes will continue. A second project is directed at combining a differential mobility analyzer (DMA) with both QqTOF and triple quadrupole mass spectrometers. Working in collaboration with Yale University, we have developed an efficient interface between the DMA and the MS, and have worked to demonstrate the improved signal-to-noise in real analytical scenarios, including LC/MS/MS analyses of biological samples such as urine extracts. The Yale DMA, with a resolution of >50, is able to separate isomers in many situations.

Dr. Wilson's research group focuses on the role of transient intermediates in enzymology and protein folding. These intermediates are crucial players in the biological activity of proteins, but quite challenging to study directly because they are i) short lived and ii) weakly populated at equilibrium. We therefore apply a broad range of analytical tools in our research including some unique MS-based approaches and biophysical NMR. We also develop new analytical technologies, including mass spectrometry coupled microfluidic devices, to enable our studies on transient intermediates. As an early career scientist, Dr. Wilson has cultivated a broad-based research record that includes publications in Protein Folding, Enzyme Kinetics, Microfluidics, Mass Spectrometry and Nuclear Magnetic Resonance as well as a US Patent. He is currently funded via the CFI Leader's Opportunity Fund.

Refereed Publications 2007-2008

1. Ions in Space. Simon Petrie and Diethard K. Bohme, Mass Spectrometry Reviews 26, 258-280 (2007).

2. Ion-Mobility Study of Two Functionalized Pentacene Structural Isomers Using a Modified Electrospray/Triple Quadrupole Mass Spectrometer. Svitlana V. Shcherbyna, Vladimir I. Baranov, Diethard K. Bohme, Christopher R. Swartz, John E. Anthony, Int. J. Mass Spectrom. 261, 45-52 (2007).

3. An investigation of the dissociation of complexes of triethylene tetramine with first-row transition-metal dications by electrospray ionization tandem mass spectrometry: remote C-C bond activation. Janna Anichina, Diethard K. Bohme, Int. J. Mass Spectrom. 267, 256-262 (2007).

4. A novel chemical reactor suited for studies of biophysical chemistry: construction and evaluation of a selected ion flow tube utilizing an electrospray ion source and a triple quadrupole detection system" Gregory K. Koyanagi, Vladimir I. Baranov, Scott D. Tanner, Michael J. Y. Jarvis, Stefan Feil, Diethard K. Bohme. Int. J. Mass Spectrom. 265, 295-301 (2007).

5. Gas-Phase Synthesis of Amino Acids: Beta versus Alpha. Jamie L. Snow, Galina Orlova, Voislav Blagojevic, Diethard K. Bohme. J. Am. Chem. Soc.129, 9910-9917 (2007).

6. Scrubbing ions with molecules: kinetic studies of chemical noise reduction in mass spectrometry using ion-molecule reactions with dimethyl disulfide. Michael J. Y. Jarvis, Gregory K. Koyanagi, Xiang Zhao, Thomas R. Covey and Diethard K. Bohme. Analytical Chemistry 79, 4006-4012 (2007).

7. Gas-phase Formation of Radical Cations of Monomers and Dimers of Guanosine by Collision-Induced Dissociation of Cu(II)-Guanosine Complexes. Ping Cheng and Diethard K. Bohme. J. Phys. Chem. B, 111, 11075-82 (2007).

8. Heavy Water Reactions with Atomic Transition-Metal and Main-Group Cations: Gas-Phase Room-Temperature Kinetics and and Periodicities in Reactivity. Ping Cheng and Diethard K. Bohme. J. Phys. Chem. A, 111, 8561-8573 (2007).

9. Ozone Reactions with Alkaline-Earth Metal Cations and Dications in the Gas Phase: Room-Temperature Kinetics and Catalysis. Stefan Feil, Gregory Koyanagi, Al Viggiano, Diethard K. Bohme, J. Phys. Chem. A, 111, 13397-13402 (2007).

10. Gas-Phase Observation of the Heterolytic Dissociation of Negative Ions into Counter Ions: Dissociation of [Cu phthalocyanine $(SO_3)_4Na]^{-3}$. Sara Hashemi, Michael J. Y. Jarvis and Diethard K. Bohme, J. Am. Soc. Mass Spec., 19, 375-379 (2008).

11. Packing atomic metal cations with C_{60}: mass spectrometric observation of $M^+(C_{60})_n$ with M = Sr and Mo and n = 0 to 4. Gregory K Koyanagi, Jianxun Xu and Diethard K. Bohme, Chem. Phys. Letters, 450, 238-241 (2008).

12. CIC Award Lecture: Gaseous Ions and Chemical Mass Spectrometry. Diethard K. Bohme, Can. J. Chem., 86, 177-198 (2008).

13. Competitive Activation of C-H and C-X Bonds in Reactions of Pt^+ with CH_3X (X=F,Cl): Experiment and Theory. Xiang Zhao, Alan C. Hopkinson, Diethard K. Bohme, ChemPhysChem 9, 873-881 (2008).

14. On the chemical resolution of the $^{87}Rb^{+}$ (s^{0}) / $^{87}Sr^{+}$ (s^{1}) isobaric interference: a kinetic search for an optimum reagent. Ping Cheng, Gregory K. Koyanagi and Diethard K. Bohme, Analytica Chemica Acta, 627, 148-153 (2008).

15. Structures, fragmentation and protonation of trideoxynucleotide CCC mono- and dianions. Janna Anichina, Stefan Feil, Einar Uggerud, Diethard K. Bohme, J. Am. Soc. Mass Spec. 19, 987-996 (2008).

16. Dissociative electron attachment to DNA bases near absolute zero: freezing dissociation intermediates. S. Denifl, F. Zappa, A. Mauracher, F. Ferreira da Silva, A. Bacher, O. Echt, T.D. Märk, D.K. Bohme and P. Scheier. Chem. Phys. Chem. 9, 1387-1389 (2008).

17. Isotope effects in dissociative electron attachment to the DNA base thymine, S. Denifl, P. Sulzer, F. Zappa, S.Moser, B. Kräutler, O. Echt, D.K. Bohme, T.D. Märk, Paul Scheier, Int. J. Mass Spectrom., accepted June 9, 2008.

18. Chemical Stability and Reactivity of Deprotonated Oligonucleotides (DNA) in the Gas Phase: Protonation and Solvation with Hydrogen Bromide. S. Feil, G. K. Koyanagi, J. Anichina, D.K. Bohme. J. Phys. Chem. B, 112, 10375-10381 (2008).

19. Absolute partial cross sections and kinetic energy analysis for the electron impact ionization of ethylene. N. Endstrasser, F. Zappa, A. Mauracher, A. Bacher, S. Feil, D.K. Bohme, P. Scheier, M. Probst and T. D. Märk, Int. J. Mass Spectrom., accepted June 10, 2008.

20. Heavy water reactions with alkaline-earth metal dications in the gas phase: kinetics at room temperature. S. Feil, G. K. Koyanagi, D.K. Bohme, Int. J. Mass Spectrom., accepted June 23, 2008.

21. Catalytic Oxidation of H_2 by N_2O in the Gas Phase: O-Atom Transport with Atomic Metal Cations. V. Blagojevic, A. Bozovic, G. Orlova, D.K. Bohme, J. Phys. Chem. A, accepted July 16, 2008.

22. "Helmut Schwarz zum 65. Geburtstag", Diethard K. Böhme and Detlef Schröder, Deutsche Bunsen-Magazin 10. Jahrgang 3, 113-114 (2008).

23. Yan Sun and R. Fournier, "Geometric and Electronic Structure of Closed-Shell Bimetallic A_4B_12 Clusters", Phys. Rev. A 75 (2007) 063205.

24. R. Fournier, "Trends in Energies and Geometric Structures of Neutral and Charged Aluminum Clusters", J. Chem. Theory and Comput. 3 (2007) 921--929.

25. J.Z. Guo, J.M. Goodings, and A.N. Hayhurst. What are the main gas-phase species formed by aluminum when added to a premixed flame? Combust. Flame 150, 127-136 (2007).

26. Coordination of Triply Charged Lanthanum in the Gas Phase: Theory and Experiment. T. Shi, A.C. Hopkinson and K.W.M. Siu, Chem. Eur. J., 13, 1142-1151 (2007).

27. Identification of Secreted Proteins during Skeletal Muscle Development. X.C.Y. Chan, J.C. McDermott and K.W.M. Siu, J. Proteome Res., 6, 698-710 (2007)

28. Endometrial Carcinoma Biomarker Discovery and Verification Using Differentially Tagged Clinical Samples with Multidimensional Liquid Chromatography and Tandem Mass Spectrometry. L.V. DeSouza, J. Grigull, S. Ghanny, V. Dubé, A.D. Romaschin, T.J. Colgan and K.W.M. Siu, Mol. Cell. Proteomics, 6, 1170-1182 (2007).

29. Identification of Candidate Biomarker Proteins Released by Human Endometrial and Cervical Cancer Cells Using Two-Dimensional Liquid Chromatography / Tandem Mass Spectrometry. H. Li, L.V. DeSouza, S. Ghanny, W. Li, A.D. Romaschin, T.J. Colgan and K.W.M. Siu, J. Proteome Res. 6, 2615-2622 (2007).

30. Verification of Endometrial Tissue Biomarkers Previously Discovered Using Mass-Tagging and Multidimensional Liquid Chromatography / Tandem Mass Spectrometry by means of Immunohistochemistry in a Tissue Microarray Format. V. Dubé, J. Grigull, L.V. DeSouza, S. Ghanny, T.J. Colgan, A.D. Romaschin and K.W.M. Siu, J. Proteome Res. 6, 2648-2655 (2007).

31. Gas-Phase Fragmentation of Protonated Benodiazepines. Risoli, J.B.Y. Cheng, U.H. Verkerk, J. Zhao, G. Ragno, A.C. Hopkinson and K.W.M. Siu, Rapid Commun. Mass Spectrom., 21, 2273-2281 (2007).

32. Endogenous Peptides from Biophysical and Biochemical Fractionation of Serum Analyzed by Matrix-Assisted Laser Desorption/Ionization and Electrospray Ionization Hybrid Quadrupole Time-of-Flight Mass Spectrometry. M. Tucholska, S. Scozzaro, D. Williams, S. Ackloo, C. Lock, K.W.M. Siu, K.R. Evans and J.G. Marshall, Anal. Biochem., 370, 228-245 (2007).

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Any Changes in Physical Space at the Unit.

None

List of all Contractual Obligations Entered into By or on Behalf of the Unit

No.