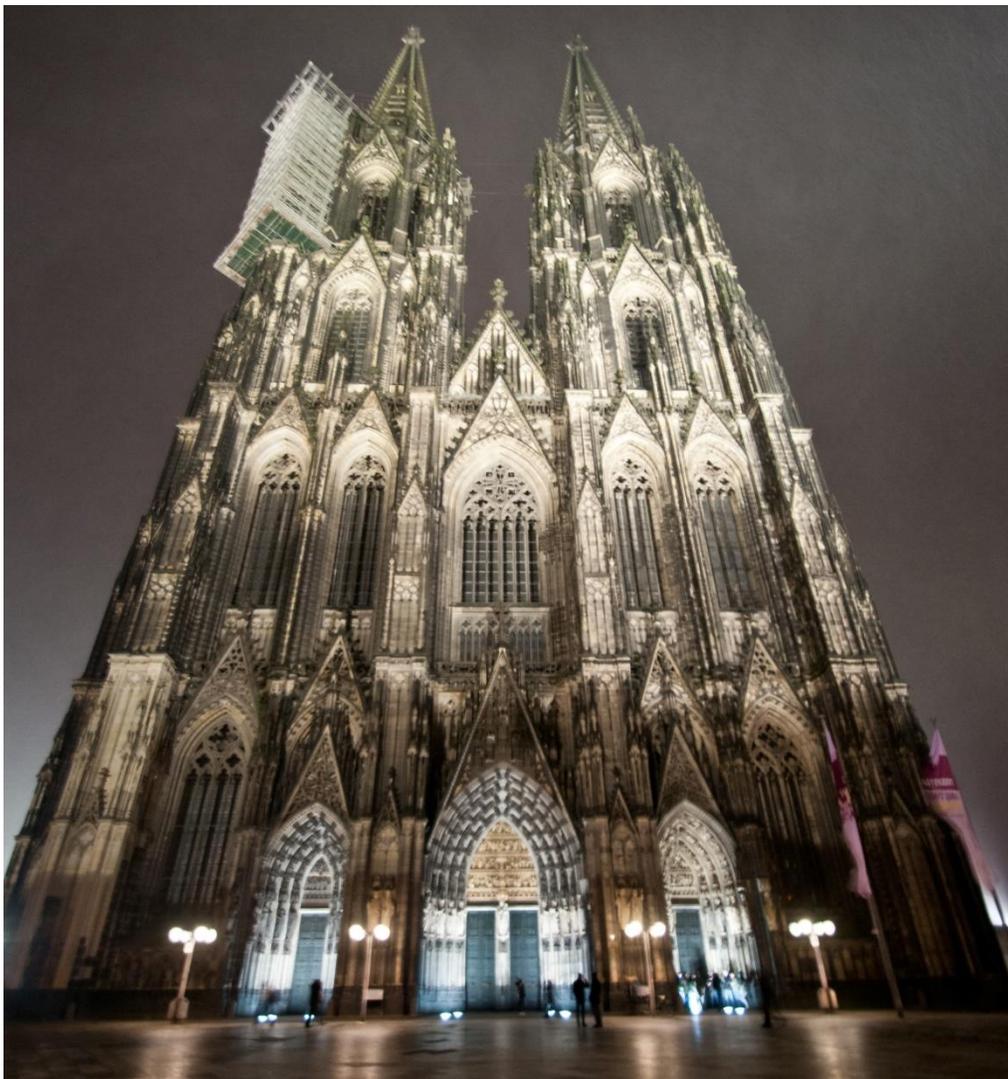




EUROHEMS2018

COLOGNE, GERMANY OCTOBER 16-18, 2018

12th Workshop on Harsh Environment Mass Spectrometers
Presented by INFICON Inc.



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THANK YOU FOR ATTENDING!

On behalf of the HEMS board of directors I want to thank you for participating in the **12th Workshop on Harsh-Environment Mass Spectrometry (HEMS)**! I have visited Cologne many times for work and I absolutely love this city. I always feel welcome here and I always have a great time. Of course I also come here for work and my trips have been very productive. I wish the same for all of us attending this workshop. I want us to enjoy the conference and the city but to also have a very productive meeting.

It can be difficult being completely open with each other at times. Those of us who work in industry always have to worry about trade secrets and intellectual property. I personally believe that we're all better off concentrating on just growing mass spectrometry. Improving the technology and expanding into new markets will eventually help everyone. This workshop is about sharing experiences so that we all get better.

Tim Short started the workshop in 1999. He wanted to have the conference on a beach so everyone could relax and be comfortable sharing information. Beachwear, including shorts, was almost mandatory. October in Cologne is probably not beach weather but I want to be clear about the dress code for the conference. It's casual. No suits or ties please!

We have a great program that can only be improved when we talk we each other. There will be plenty of time to interact and I look forward to reconnecting with old friends and meeting new people. See you all in Cologne!

Danke!

Ken Wright
Organizer of EUROHEMS2018 and HEMS Board Member
Ken.wright@inficon.com

History of the HEMS Workshop

The Harsh-environment Mass Spectrometry (HEMS) Workshop was created in 1999 as a means of encouraging interaction among people involved in deploying mass spectrometers outside of the typical laboratory setting. These environments are diverse, ranging from volcanoes and battlefields, to ocean depths, outer space and other rugged locales. Building mass spectrometers to withstand the rigors of such harsh and remote environments places a unique burden on engineering design and science objective planning, where operational requirements for power, size, and durability must be met while achieving the goals of the scientific mission. We hope to foster and promote interaction between scientists and engineers through the informal setting of the HEMS Workshop and thus stimulate the development of HEMS technology and applications.

Previous Workshops

1st Workshop on Harsh Environment Mass Spectrometers

February 21-23, 1999; St. Petersburg, Florida

Sponsored by the University of South Florida, Marine Science Department, Center for Ocean Technology

2nd Workshop on Harsh Environment Mass Spectrometry

March 18-21, 2001; St. Petersburg, Florida

Presented by the University of South Florida, Marine Science Department, Center for Ocean Technology

The 3rd Harsh-Environment Mass Spectrometry Workshop & The 2nd NASA/JPL Miniature Vacuum Pumps Workshop

March 25-28, 2002; Pasadena, California

Presented by the Jet Propulsion Laboratory/NASA

The 4th Harsh-Environment Mass Spectrometry Workshop

October 7-10, 2003; St. Petersburg, Florida

Presented by the Center for Ocean Technology, University of South Florida College of Marine Science

The 5th Harsh-Environment Mass Spectrometry Workshop

September 20-23, 2005; Lido Beach, Sarasota, Florida

Presented by the Center for Ocean technology, University of South Florida College of Marine Science

The 6th Harsh-Environment Mass Spectrometry Workshop

September 17,20, 2007; Cocoa Beach, Florida

Presented by the ASRC Aerospace Corporation, Kennedy Space Center

The 7th Harsh-Environment Mass Spectrometry Workshop

September 21-24,2009; Santa Barbara, California

Presented by the Hamilton Sundstrand Corporation

The 8th Harsh-Environment Mass Spectrometry Workshop

September 19-21, 2011; St. Pete Beach, Florida

Presented by the University of North Texas

The 9th Harsh-Environment Mass Spectrometry Workshop

September 15-18, 2013; St. Pete Beach, Florida

Presented by the University of North Texas

The 10th Harsh-Environment Mass Spectrometry Workshop

September 13-16, 2015; Baltimore, Maryland

Presented by OI Analytical

The 11th Harsh-Environment Mass Spectrometry Workshop

September 18-21, 2017; Oxnard, California

Presented by UTC Aerospace Systems

For programs, proceedings, and participants please visit: <http://www.hems-workshop.org/Archive.html>

2018 Organizing Committee

12th HEMS: Ken Wright

Abstracts: Tim Short, Steve Taylor

Student Awards: Torben Gentz

Corporate Sponsors: Guido Verbeck

Registration/Program: Lynell DeWind

Website: Strawn Toler

LinkedIn Advertising: David Vincett

Student Award Winners

Ifeoluwa Ayodeji

Department of Chemistry, University of South Florida

Dalton Snyder

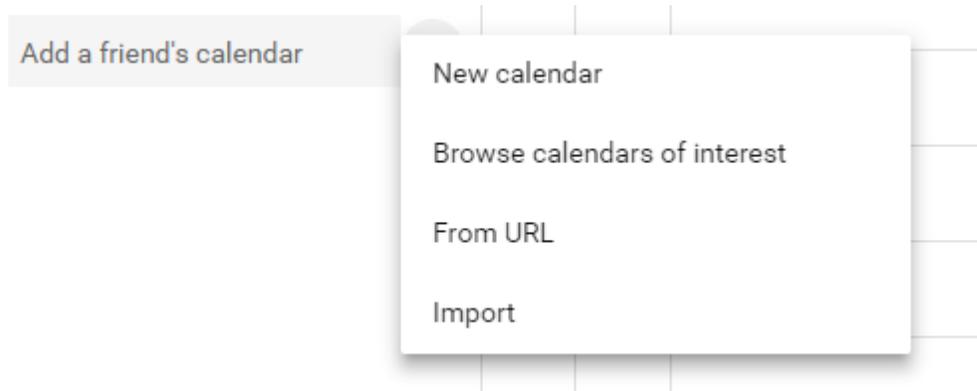
Department of Chemistry, Purdue University

GOOGLE CALENDAR

We are trying something new this year in an attempt to be a little more environmentally friendly. **There will be no printed program handed out for this workshop.** Instead, there is a Google calendar that you can use to access the schedule and abstracts. It also contains map locations for the hotel and Workshop dinner as well as menus for the opening reception and dinner. Just click on any item in the calendar and more information will pop-up. Keep in mind the calendar is in local Cologne time!

Google Calendar users:

You can add a calendar by selecting “Add a friend’s calendar” and “From URL” and then just past the EUROHEMS2018 calendar URL when prompted.



EUROHEMS2018 calendar URL:

https://calendar.google.com/calendar/embed?src=217hiod5bjugdaimc8hcer86ng%40group.calendar.google.com&ctz=America%2FNew_York

You can also paste the above URL into a browser. If you select “Agenda” mode instead of “Week” or “Month” it will look quite good.

iPhone Users can use the iCal Format

EUROHEMS2018 calendar URL iCal:

<https://calendar.google.com/calendar/ical/217hiod5bjugdaimc8hcer86ng%40group.calendar.google.com/public/basic.ics>

PROGRAM

PRESENTATIONS are 20+ min (please leave 5 to 10 min for discussion)

	EUROHEMS2018 Workshop – OCTOBER 16
6 – 8 PM	Registration and Opening Reception. Outside Saal 2 Heumarkt, Maritim Hotel

	EUROHEMS2018 Workshop – OCTOBER 17
7 – 8:30 AM	Set-up of Vendor Tables and Registration
9:00 AM	Welcome Remarks and Vendor Introductions
10:00 AM	<i>“Anomalous Uses of Mass Spectrometers at NASA”</i> Kathleen B. Loftin, Ph.D., Deputy Center Chief Technologist, NASA Kennedy Space Center
10:30 AM	Mid-Morning Break
11:00 AM	Technical Session I <i>“Development of Portable Mass Spectrometer for Explosives and Narcotics Detection”</i> Vadym Berkout, Smiths Detection
11:30 AM	<i>“CubeSat QIT-MS: Rad Hard Miniature Instrument for Solar System Exploration”</i> Stojan Madzunkov, Jet Propulsion Laboratory
12:00 PM	Buffet Lunch Provided
1:30 PM	Technical Session II <i>“An optimized membrane inlet system (MIS) for underwater mass spectrometry (UWMS).”</i> Malte Höhn, Christian Hamm, Justin Chaillot, Marvin Frank, Torben Gentz Alfred-Wegener-Institute for Polar and Marine Research
2:00 PM	<i>“Isotopic ratio study of uranyl ion with Differential mobility Spectrometry-mass spectrometry (DMS-MS)”</i> Ifeoluwa Ayodeji and Theresa Evans-Nguyen, Dept. of Chemistry, University of South Florida Sunil Badal, Garrett Maclean and Jacob T. Shelley, Dept. of Chemistry and Chemical Biology Rensselaer Polytechnic Institute
2:30 PM	Mid-Afternoon Break
3:00 PM	Technical Session III <i>“Triode-type MCP-based Ion Detector Enabling Miniature Mass Spectrometers to Operate at Higher Pressure up to 1Pa”</i> Masahiro Hayashi, Yuuya Washiyama, Kentaro Ishii and Joji Sakakiyama, Hamamatsu Photonics K.K., Hamamatsu
3:30 PM	<i>“Field Deployable Mass Spectrometers at ToFwerk”</i> Marc Gonin, TOFWERK
4:00 PM	<i>“Optimization of a portable QMS for environmental monitoring”</i> T. Fildes, D.G. McIntosh, M.J. Antony Joseph, B. Smith, S. Maher, J.R. Gibson and S. Taylor Department of Electrical Engineering and Electronics, University of Liverpool
4:30 PM	End of Day 1
7:00 PM	Workshop Dinner - 

	EUROHEMS2018 Workshop – OCTOBER 18
9:00 AM	Technical Session IV
	<i>“Rapid Identification of Drug Seizures by ASAP-MS on a Low-Cost, Deployable, Single Quadrupole Instrument”</i> Bryan McCullough, Chris Hopley, National Measurement Laboratory, LGC David Douce, Nicola Lumley, Steve Bajic and Kate Whyatt, Waters Corporation
9:30 AM	<i>“Mobile Mass Spectrometer Systems for Online Oil Emission and Oil Dilution Measurements in Combustion Engine Test Cells.”</i> Andreas Behn, Matthias Feindt, Sven Krause, Lars Schomann, Lubrisense GmbH Ann-Christin Preuss, Gerhard Matz, Institute of Analytical Measurement Technology Hamburg
10:00 AM	Mid-Morning Break
10:30 AM	Technical Session V
	<i>“Two-dimensional mass spectrometry on benchtop and portable ion trap mass spectrometers”</i> Dalton Snyder, Lucas Szalwinski, Ryan Hilger, Robert Schrader, Valentina Pirro, R. Graham Cooks, Purdue University Department of Chemistry Zachary St. John, The College of New Jersey, Desmond Kaplan, KapScience LLC, Ryan Danell, Danell Consulting, Inc., Veronica Pinnick, Paul Mahaffy, NASA Goddard Space Flight Center, Mitch Wells, FLIR Systems, Inc
11:00 AM	<i>“Development of Micro-Time-Of-Flight Mass Spectrometer for in situ gas analysis”</i> Alexandre Sonnette, Frédéric Progent, Jérôme Tupinier, Pierre-Etienne Buthier, Jean-Christophe Lictevout, Sébastien Vigne, CEA, DAM, DIF Thomas Alava, CEA, LETI, MINATEC Campus
11:30 AM	<i>“Instrumentation for Lunar Volatile Analysis”</i> Janine Captain, NASA Kennedy Space Center
12:00 PM	Buffet Lunch Provided
1:30 PM	Technical Session VI
	<i>“Development of a robust Fourier-Transform ion trap for semiconductor manufacturing”</i> Valerie Derpmann, Yessica Brachthäuser, Rüdiger Reuter, Michel Aliman, Alexander Laue, Hin Yiu Chung, Carl Zeiss SMT GmbH
2:00 PM	<i>“Reverse-gas stack modeling-coupled to fieldable mass spectrometry to locate chemical effluent streams for clandestine drug labs, explosives manufacturing, and chemical weapon deployment.”</i> Guido F. Verbeck, Camila Anguiano Virgen, University of North Texas Kenneth C. Wright, Jaime L. Winfield, James D. Fox, INFICON Inc
2:30 PM	<i>“Evaluation of Portable Linear Ion Trap Mass Spectrometer Coupled to Paper Spray Ionization Source for the Detection of Chemical Warfare Agents”</i> Ethan M. McBride, Phillip M. Mach, Elizabeth S. Dhummakupt, Trevor Glaros Daniel O. Carmany, Paul S. Demond, Gabrielle R. Boyd, Excet, Inc
3:00 PM	Mid-Afternoon Break
3:30 PM	Technical Session VII - Continued on next page

3:30 PM	Technical Session VII <i>"A Quadrupole Ion Trap for the Detection of Biomarkers at Icy Worlds"</i> Joshua Wiley, Anton Belousov, Sarah Waller, Dragan Nikolic, Richard Kidd, Stojan Madzunkov, Morgan Cable, Murray Darrach Jet Propulsion Laboratory, California Institute of Technology
4:00 PM	<i>"Optimization of a drone based miniature mass spectrometer system (Drone-MS) for in situ gas plume measurements"</i> Jorge Andres Diaz, Ernesto Corrales, David Diaz, Alfredo Alan, GasLAB, CICANUM. Physics School. Universidad de Costa Rica, Kenneth Wright, INFICON Inc., Robert Kline-Shoder, CREARE Inc., David Pieri, Jet Propulsion Laboratory, California Institute of Technology
4:30 PM	Program Survey and Closing Remarks
5:00 PM	Evening Free – Informal Old City Tours!

RECEPTION & REGISTRATION

TUESDAY, OCTOBER 16, 6-8 PM

LOCATION: Outside the meeting room, Saal 2 Heumarkt

S TARTERS

Mixed, assorted lettuce
Yoghurt dressing, oil and vinegar
Stripes of cheese and ham

Chicken with curry and fruits
Graved salmon, horseradish cream
Salad of cucumber and alga

Cream soup of leeks and potatoes
Bread croutons

M AIN COURSE

Stripes of pork Zurich style
Coalfish meunière style
with bacon and shrimp
Swabian pasta and small potatoes

D ESSERT

Grits of red fruits, vanilla sauce
Chocolate mousse
Fruit salad

Bread rolls with salted butter

ABSTRACTS

1

Anomalous Uses of Mass Spectrometers at NASA

Kathleen B. Loftin, Ph.D

Deputy Center Chief Technologist, NASA Kennedy Space Center

At the Harsh Environment Mass Spectrometer workshop we focus on bringing the Mass spectrometer to the sample because it's not practical to bring the samples back to the laboratories. However there are many NASA mass spectrometer applications where we bring the samples to the instrument. This presentation will discuss some of those applications that are ripe for innovative instrument development

Development of Portable Mass Spectrometer for Explosives and Narcotics Detection

Vadym Berkout
Smiths Detection

Introduction

Mass spectrometry (MS) has the potential to improve trace detection for security applications through improved selectivity, greater threat library size and availability of additional information provided by MS/MS analysis. The improvements offered by MS increase reliability of detection, thus minimizing requirements for secondary searches, and should also significantly reduce false alarms.

Methods

The MS prototype is based on a linear ion trap (LIT) analyzer with atmospheric pressure (API) interface. To achieve efficient ion transmission with a small vacuum system a novel ion funnel design was implemented. Sampling methodology that is currently in use by security professionals such as TSA screeners is based on swab collection. A thermal desorber (TD) interfaced to the LIT analyzer is used to liberate sample from the surface-sampling swabs. Desorbed sample vapors are ionized using a dielectric-barrier discharge (DBD). Testing of the TD-MS system is performed by depositing explosive and narcotic standards on swabs.

Preliminary Data

Analytical figures-of-merit, including sensitivity and selectivity, will be presented to demonstrate the capability of the system for detecting trace levels of target explosives and narcotics.

Novel Aspect

A portable mass spectrometer with an efficient API interface developed to meet security checkpoint functional and analytical requirements is described.

CubeSat QIT-MS: Rad Hard Miniature Instrument for Solar System Exploration

Stojan Madzunkov
Jet Propulsion Laboratory, Pasadena, CA

We present a new miniaturized mass spectrometer prime rely designed for sampling the atmospheres of the planetary bodies of the Solar System. The sensor is based on our previous 10mm Quadruple Ion Trap (QIT) design [1, 2] but with many improvements such as smaller sensor size, less power consumption, new electronics design etc. However, the new sensor has the same measuring capabilities. This is a cube-sat compatible instrument consisting of multiple 4"x4"x4" (U) units. The electronics for this instrument is designed from scratch in collaboration with Caltech and Space Physics Research Lab. The electronics is fully vacuum compatible and designed with rad-hard flight-like parts with utilizing technology and experience of preceding NASA missions. The size of electronics is 3U with components nominally rated for up to 100 krad. The electronics is made out of 5 main boards: digital control board (which is not rad hardened at the moment), power distribution unit (100 – 300krad), analog control and telemetry board (100krad), mass spectrometer control board (100-300krad) and RF power amplifiers (300krad). The sensor is based on the low capacitance (30pF) 8 mm QIT. The electron optics, detector and the sensor are housed within custom 3D printed titanium vacuum chamber and have been tested for vibration loads up to 60G. Sensor with pumping system occupies another 5U. Heat sink and radiation shielding is implemented for sensitive components and may be additionally reinforced to ensure stable operation during various planetary missions. The instrument mass is estimated at 6 kg and it requires 30W of power for nominal operation.

[1] Madzunkov et al., Accurate Xe Isotope Measurement Using JPL Ion Trap, J. Am. Soc. Mass Spectrom. (2014) 25:1841Y1852

[2] Madzunkov et al., Progress Report on the Spacecraft Atmosphere Monitor, 46th International Conference on Environmental Systems, 10-14 July 2016, Vienna, Austria

An optimized membrane inlet system (MIS) for underwater mass spectrometry (UWMS)

Malte Höhn, Christian Hamm, Justin Chaillot, Marvin Frank, Torben Gentz
Alfred-Wegener-Institute for Polar and Marine Research, Bremerhaven, Germany

The pressure resistance in the deep ocean is most important for in-situ measurements. In case of the underwater mass-spectrometry (UWMS) especially the requirements of the combination of high permeability for fast low detection limits and stable structures for pressure resistance in the membrane-inlet-systems (MIS) are challenging. In the third funded project "SensorEplus" a MIS is redesigned and optimized to get high pressure resistance with high gas permeability.

The specific details in this project are pressure stability of up to water depth of 4000 m (400 bar), and a high porosity of the membrane supporting structure for gases to get low limits of detection for several gases and chemicals.

While comparing these requirements with natural structures of diatoms in the ELISE department of the AWI-Bremerhaven (<http://elise.de/en/>), it was found a design solution: a kind of tree stabilization inside of the "German Frit" with a very porous surrounding surface. The designed component has a cylindrical form with a diameter of 1/8" at a length of 13 mm. To realize the production of a small and complex component like this, the manufacturing process of micro-printing as a generative manufacturing is used.

Additionally a new heating management is adapted in the redesigned MIS. By heating the membrane a constant temperature is achieved and potentially energy can be saved. Also the use of a heat exchanger enables a constant temperature while saving energy.

To check the stability of the MIS the components are tested in a high pressure tank at the AWI facilities to prevent a failure of each component. The permeability of the new developed MIS will be tested with the AWI-UWMS to get a comparison of the old MIS supported by a spring and the new structure.

Here, we will present the evolution process and the structure of the new "German Frit".

Isotopic ratio study of uranyl ion with Differential mobility Spectrometry-mass spectrometry (DMS-MS)

Ifeoluwa Ayodeji and Theresa Evans-Nguyen

Department of Chemistry, University of South Florida, Tampa, Florida

Sunil Badal, Garrett Maclean and Jacob T. Shelley

Department of Chemistry and Chemical Biology, Rensselaer Polytechnic Institute, Troy, NY

Introduction:

The human threat associated with radio-nuclear materials from nuclear fuel feedstock, spent fuel and post detonation debris require a rapid and high throughput analytical approach. Isotope-ratio mass spectrometer (IRMS) – with a magnetic sector analyzer is the conventional instrument employed for IR measurement. The size, weight and power (SWP) requirements of the lab-based instrument makes sampling and analysis laborious and time consuming. Deploying differential mobility spectrometry (DMS) system will reduce the sampling time to order of milliseconds. With the heterogeneous nature of fission products, DMS ion filtration prior to MS analysis will reduce chemical interference while ion of interest is selectively characterized. Herein, we will focus on the DMS filtration of uranyl ion from its salts and further conduct an isotopy-ratio study on selected ion.

Method:

Uranyl nitrate salt, acetyl-acetonate or tributyl phosphate complexed solution were nanosprayed at 1 $\mu\text{L}/\text{min}$. Ions are filtered through 0.5 mm gap between two electrodes (15 mm \times 4 mm) of a home-built DMS cell, interfaced to a commercial trap MS (Thermo LTQ-XL). The rf and dc potential were supplied to the DMS electrodes by a commercial Sionex electronic.

Preliminary Data:

A plasma-based ionization technique; Flowing atmospheric pressure after-glow (FAPA) was initially employed. While DMS method was set to scan dispersion voltages (DV) and compensation voltages (CV) within ~ 5 minutes, uranyl acetylacetonate ion $[[\text{UO}_2(\text{AcAc})_2+\text{H}]^+]$ was filtered out at a fixed DV and CV of 1000 V and -1.86 V, respectively. MS/MS of the filtered complexed ion produces uranyl ion (UO_2^+ ; m/z 270). Hence, isotopy studies were performed on UO_2^+ . At DMS off and on, the $^{235}\text{U}/^{238}\text{U}$ ratio; SD; RSD were 0.00705; 4.25×10^{-4} ; 5.9 % and 0.00727; 1.43×10^{-4} ; 2.0 %, respectively. This result indicates that DMS is a promising analytical tool for isotopy measurement. For further investigation, we shall explore a continuous ionization source including nanospray for sample in solution; and a laser desorption-atmospheric pressure chemical ionization (LD-APCI) for surface ionization.

Novel Aspect: Nuclear forensic, isotopy ratio measurement, ambient ionization, differential mobility spectrometry for rapid screening of radionuclear debris.

Triode-type MCP-based Ion Detector Enabling Miniature Mass Spectrometers to Operate at Higher Pressure up to 1Pa

Masahiro Hayashi, Yuuya Washiyama, Kentaro Ishii and Joji Sakakiyama,
Hamamatsu Photonics K.K., Hamamatsu, JAPAN

Recent interest in portable mass spectrometry applications has spurred a great deal of research into the development of miniature mass spectrometers (MS) such as desktop type explosives trace detectors (ETDs). In the near future, there is a possibility that ETDs used at checkpoint screening will change from the current ones based on ion mobility spectrometers to ones based on next-generation MS.

In order to retain the major advantage of portability, miniature MS systems typically use small vacuum pumps with relatively low pumping speeds, meaning the miniature MS has to be operated at relatively low vacuum levels ($>1e-2$ Pa). Also in terms of sensitivity and vacuum condition, almost all miniature MS systems under development have adopted the ion trap analyzer. In these system configurations, ion detectors are required to have both higher pressure operation ($>1e-2$ Pa) and high gain ($>1e+6$). Currently, channel electron multipliers (CEM) are mainly used in miniature MS, but it is difficult for CEM to satisfy the required specifications.

Conventional electron multiplier based detectors including CEM and microchannel plates (MCP) cannot be adapted to operate at low vacuum ($>1e-2$ Pa) because of ion feedback (IFB), which causes discharges and decreases in S/N. However, the reduced dimensions of a typical MCP detector, which can be less than the mean free path in conventional electron multiplier based detectors, make it suitable for higher pressure operation. The major source of IFB, which is a peculiar phenomenon of secondary electron amplification, was found to be the creation of ions from residual gas molecules.

We concluded that controlling the residual gas ions is more important than suppressing the ion generation. In order to realize this idea, we introduced a triode structure into the conventional MCP detector to enable it to operate at higher pressure condition. A compact detector for miniature MS could be realized by simplifying the structure in terms of supply voltage conditions and achieves the target gain of $1e+6$ at 1Pa. We will confirm the MCP detector operation in a higher pressure region by improving the current evaluation system, and optimize the MCP detector for a commercialized MS.

Field Deployable Mass Spectrometers at Tofwerk

Marc Gonin

TOFWERK Thun, Switzerland

Tofwerk has a long history in field deployable instruments. This started with the PhD work of the founders and continued with instruments for atmospheric sciences and now propagates into other fields.

Several deployable instruments will be presented.

1. An ion mobility spectrometer-mass spectrometer (IMS-MS) that was run continuously for multiple weeks at a remote Alabama field site during the 2013 Southern Oxidant and Aerosol Study (SOAS) campaign;
2. A chemical ionization mass spectrometer (CI-MS) installed aboard the aircraft NSF/NCAR C-130 in special frames that can withstand turbulent conditions for Wintertime INvestigation of Transport, Emissions, and Reactivity (WINTER 2015) campaign. Inlets mounted through the wall of the aircraft sample air directly from the sky into the mass spectrometers for the measurement of trace gases;
3. A fully customized compact TOF aboard the M55-Geophysica aircraft carrying instruments to stratospheric altitudes.

The requirements and technology will be discussed. Finally, some of the lessons that have been learned are discussed.

Optimization of a portable QMS for environmental monitoring

T. Fildes, D.G. McIntosh, M.J. Antony Joseph, B. Smith, S. Maher, J.R. Gibson and S. Taylor
Department of Electrical Engineering and Electronics, University of Liverpool
Brownlow Hill, Liverpool L69 3GJ

The use of small portable MS instruments offers many advantages for environmental studies including in-situ detection and monitoring of stable and unstable isotopes in real time in field conditions. However the use of smaller instruments brings its own challenges of reduced sensitivity, resolution and stability. In this work we assess by 3D simulation the effect of the QMS pre-filter, electrode bias (pole bias) and ion source geometry on instrument resolution and stability. Of particular interest is the ion source to mass filter gap distance on ion coupling into the mass filter. The simulations are supported by experimental measurements on portable single filter, dual and triple filter QMS instruments. The focus of this combined approach is the instrument optimization so as to obtain the best possible performance in the smallest possible package. The application for this work is stable isotope analysis (including $\delta^{15}\text{N}$ and $\delta^{13}\text{C}$) for environmental monitoring (underwater and in ambient), for isotopic tracer measurements for biomedical investigations and for archaeological applications.

1. Effects of the source gap on transmission efficiency of a quadrupole mass spectrometer

Mariya J. Antony Joseph, David G. McIntosh, J. Raymond Gibson, and Stephen Taylor, *Rapid Communications in Mass Spectrometry*, 32(9), pp. 677–685 (2018)

Rapid Identification of Drug Seizures by ASAP-MS on a Low-Cost, Deployable, Single Quadrupole Instrument

Chris Hopley, Bryan McCullough, National Measurement Laboratory, LGC, Teddington, UK

David Douce, Nicola Lumley, Steve Bajic and Kate Whyatt, Waters Corporation, Wilmslow, UK

Here, we describe the development of a prototype atmospheric solids analysis probe ion source for a miniaturised MS – the Waters QDa – and its application to the characterisation of drug seizures.

The QDa is a small, low cost quadrupole MS originally designed as a simple-to-use instrument for chromatography. Its ion source was redesigned to incorporate a corona pin and to allow the insertion of a solid probe (glass capillary) The sample was desorbed from the rod using a flow of heated gas before being ionised via a corona discharge operating in fixed voltage mode. Samples were analysed in full scan mode, data was recorded in four channels using a different cone voltage in each in order to induce in-source fragmentation of the analytes to allow increased certainty of identification. Data was obtained for a large number of solvent standards covering a wide range of drugs of abuse (DoA) including amphetamines, opioids, stimulants, cathinones, cannabinoids, steroids, and legal highs; data was also obtained for a series of common cutting agents such as caffeine. This data was used to build an identification database in order to test street drug seizures.

The initial experiments were carried out using the instrument in so-called performance mode which uses a 0.2 mm inlet aperture and a free-standing rotary pump to maximise sensitivity. In order create a deployable version of the instrument it was reconfigured to 'standard' mode which uses a bolt-on diaphragm pump and a 0.09 mm diameter orifice. In addition, the nitrogen gas used for desorption in the initial experiments was changed to air with the flow generated using a small air pump eliminating the need for a dedicated gas supply. This new set-up was subsequently tested with a range of standards and seizures and shown to be an extremely powerful tool for the rapid identification of drugs of abuse.

Mobile Mass Spectrometer Systems for Online Oil Emission and Oil Dilution Measurements in Combustion Engine Test Cells

Andreas Behn, Matthias Feindt, Sven Krause, Lars Schomann
Lubrisense GmbH, Hamburg, Germany

Ann-Christin Preuss, Gerhard Matz
Institute of Analytical Measurement Technology Hamburg e.V., Hamburg, Germany

Adapting internal combustion engines to current and future emission standards requires an ever-rising effort in simulation and testing. While the combustion process itself is well known and measurable, specialized tools are necessary to minimize the effects of engine oil emission and fuel-oil-interaction. Due to dynamic test runs and the number of different runpoints and engine conditions, offline analysis or even slow sampling setups are not an option.

The combination of a compact TOF-MS with fast and robust direct inlet systems allows for a detailed quantification and analysis of engine oil HC emission in exhaust gas. The information obtained is then used to minimize the oil consumption via engine hardware and software changes, decreasing both HC and PM emission.

With the addition of a fast online GC and a multiport sampling and injector system, the measurement system can also be used for observation of dynamic fuel ingress into engine oil as well as fuel and oil aerosol emission from the crankcase.

Design, application and results of both setups in live engine test cells will be shown and discussed.

Two-dimensional mass spectrometry on benchtop and portable ion trap mass spectrometers

Dalton Snyder, Lucas Szalwinski, Ryan Hilger, Robert Schrader, Valentina Pirro, R. Graham Cooks
Purdue University Department of Chemistry, West Lafayette, IN
Zachary St. John; The College of New Jersey, Ewing Township, NJ
Desmond Kaplan; KapScience LLC, Tewksbury, MA
Ryan Danell; Danell Consulting, Inc., Winterville, NC
Veronica Pinnick, Paul Mahaffy; NASA Goddard Space Flight Center, Greenbelt, MD
Mitch Wells; FLIR Systems, Inc., West Lafayette, IN

Although miniature mass spectrometers have been the subject of intense interest for nearly two decades, they have only recently become broadly available as commercialized products. Their recent availability can be attributed to important advances in atmospheric pressure sampling, vacuum system miniaturization, mass analyzer geometry optimization, miniaturization, and simplification, and the advent of highly accessible and broadly applicable ion sources. Even with these advances, the standard configuration for portable systems is still gas chromatography coupled to electron impact ionization (GC-EI) and either a quadrupole mass filter or a quadrupole ion trap for mass analysis. Portable ambient ionization systems (e.g. Mini 12, Purdue University) using ion trap mass analyzers are just beginning to emerge as the sampling, ionization, and MS/MS limitations of GC-EI are realized. Herein we argue that the paradigm shift from GC-EI to ambient ionization-ion trap should be coupled with new MS/MS scanning capabilities that we have recently demonstrated.

We describe the next generation of scan modes for portable ion trap mass spectrometers, including 1) a full set of MS/MS capabilities normally accessible only on triple quadrupole systems in addition to 2) analytically powerful two-dimensional MS/MS (2D MS/MS) scans. Firstly, we will show that all three main MS/MS scan types – namely precursor ion scans, neutral loss scans, and product ion scans – are possible on a single portable ion trap system using a combination of orthogonal double resonance excitation and ac frequency scanning. Precursor and neutral loss survey scans should be particularly valuable for detecting classes of compounds in the field; we demonstrate detection of chemical warfare agents, explosives, fentanyl analogues and other opioids, and amphetamines using a variety of ambient ionization sources. Highly multiplexed precursor and neutral loss scans – i.e. scans which traverse multiple scans lines simultaneously - are also possible in a quadrupole ion trap. Lastly, 2D MS/MS scans, in which all MS/MS data from a sample is acquired in a single scan (rather than from a *set* of scans), will also be demonstrated on these illicit samples.

Development of Micro-Time-Of-Flight Mass Spectrometer for *in situ* gas analysis

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CEA is currently developing a micro time-of-flight (μ -ToF) mass spectrometer that can be coupled with gas chromatography and is therefore of great interest for *in situ* gas field analyzes. This device has numerous applications covering a wide range of fields such as the environment, industry, space, etc. In this regard, the device must have a small footprint, be lightweight, low power consuming and easily usable.

In order to meet these constraints, the technology of Micro Electro Mechanical Systems (MEMS) was used. The MEMS developed here consists of a 1 cm x 1 cm silicon chip for linear μ -ToF (Fig 1 A).

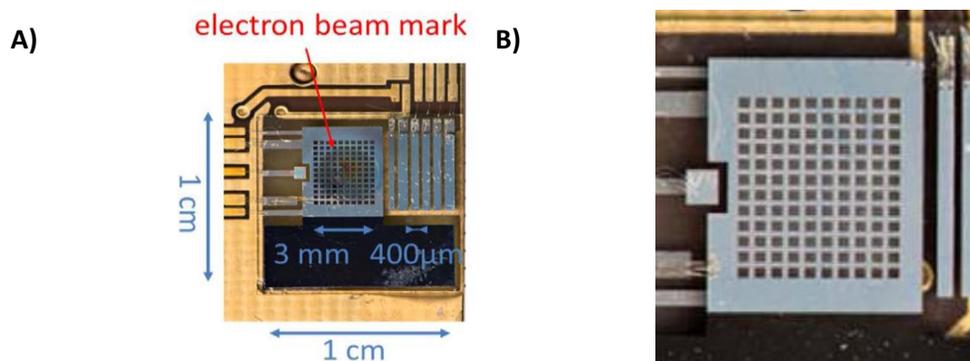


Fig. 1: A) μ -ToF ionization / extraction / focalization stage B) 3 x 3 mm grid zoom

The linear μ -ToF is composed of an ionization stage and a zone of extraction and focalization of the ions produced. In the ionization stage, the gas is bombarded through a grid (Fig 1 B) by electrons to achieve ionization by electronic impact. The electron energy is 70 eV in order to compare the results with NIST libraries. The electrons are produced thanks to a homemade electron gun using thermoionic effect. This gun has been characterized and simplified in order to obtain an intense and well-focused electron beam (2.5 mm diameter) with the minimum device size.

The extraction and focusing of the ions produced is done by means of 6 electrodes constituting electrostatic lenses whose voltages have been optimized. At the end of a time of flight, the ions are detected on a Micro Channel Plate (MCP) and the mass spectrum recorded with an oscilloscope.

Using gas mixtures of rare gas in helium we were able to obtain spectra for concentrations of 100 ppm. Effects of electrodes potentials, gas pressure and geometric layout of gas inlet were studied. This work shows encouraging results and pulls the μ -ToF one step closer towards a fully integrated portable analytical system.

Instrumentation for Lunar Volatile Analysis

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Understanding the available lunar resources is key to incorporating their availability into exploration architectures. Previous lunar missions have provided insight into the potential resources on the moon as an initial step enabling in-situ resource utilization (ISRU). Orbiting missions, such as Clementine and Lunar Prospector, have mapped the lunar polar region and found enhanced hydrogen signals on kilometer-scale resolution. The Lunar Crater Observation and Sensing Satellite (LCROSS) mission provided the first direct measurement of water ice in a permanently shadowed region. Future missions will provide ground truth data to measure and quantify lunar volatiles.

One approach to exploration capitalizes on commercial partnerships for Class D risk aware missions. Partnerships with commercial partners enable rapid design cycles, leveraging the investment of the commercial industry in instrument development. Modified Commercial off the Shelf (COTS) hardware can be utilized to enhance capabilities in exploration missions. The hardware under development at the Kennedy Space Center for availability within the Commercial Lunar Payload Services opportunities capitalizes on modified COTS, enabling an aggressive delivery schedule and low-cost development. The modified hardware has been integrated and tested in a thermal vacuum environment, with final flight modifications currently in work. The use of a modified COTS instruments will be discussed for space applications.

Development of a robust Fourier-Transform ion trap for semiconductor manufacturing

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Semiconductor manufacturing has a growing demand for in-line process control metrology as the pressure on cost efficiency and quality is steadily increasing. Especially endpoint detection is a crucial factor for etch processes, as it determines wafer throughput and quality. With shrinking node sizes and thus, decreasing open areas in etching currently used optical emission spectroscopy (OES) reaches its physical boundaries. Furthermore, the chemistry of many etch processes are not fully understood and a deeper insight would lead to process optimization. However, using mass spectrometers in etch processes can be challenging due to the aggressive chemicals used in wafer etch and chamber cleaning. This is why the main requirements for a mass spectrometer in this field are its robustness, respectively corrosion resistance and measurement speed. A Fourier Transform Ion Trap, together with a pulsed gas inlet, meets those requirements. The absence of an ion detector and the small gas load inside the instrument, together with only gold plated or ceramic surfaces lead to a high robustness against etch gases like Cl_2 , BCl_3 , HBr or HF or depositing gases like TBAs (Tetrabutylarsine) or TEGa (Triethylgallium). The sampling rate is up to 2 Hz for a full mass spectrum, which is sufficient for most processes, as typical process times are in the range of 5-20 s. The instrument has proven its applicability in etch endpoint detection, process optimization of cleaning or etch processes and process diagnostics like the understanding of first wafer effects.

Reverse-gas stack modeling-coupled to fieldable mass spectrometry to locate chemical effluent streams for clandestine drug labs, explosives manufacturing, and chemical weapon deployment

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Presented here is the fieldable automobile and backpack mass spectrometers. The front end of a Membrane Inlet Mass Spectrometer (MIMS) system incorporates three dual inlet ports allowing for differing MIMS materials and selectivity for specific environments. Membranes here have proved selective for a myriad of organic compounds as well as aromatic hydrocarbons, both nitrogen and peroxide-based explosives, chemical weapon simulants, and clandestine drugs. Recent results not only showcase the system's applicability to chemical warfare agent (CWA) detection, but its ability to identify the type of agent emitted. Performance against current field detectors has illustrated both the increase sensitivity and selectivity of the presented fieldable device.

The MIMS system is deployable and rugged which is especially significant considering the various environment conditions it's exposed to, and the numerous accoutrements such as foreline pumps and inert gas tanks required of a mass spectrometer. Further innovations include increasing sensitivity by development of a near-infrared (NIR) laser diode system for membrane desorption and enhanced permeability with high parts-per-trillion (ppt) limits of detection and rapid analysis performance just seconds after the initial time of exposure. All of these are incorporated with GIS, for position monitoring, mapping, and integrity of analysis. Software has been developed to incorporate the chemical mass mapping, reverse gas stack modeling (RGSM), and SAMs data to produce accurate point of source determination, even with simple drive-bys or stationary remote monitoring. By coupling the MIMS system with RGSM, the determination of upwind source locations of chemical weapon deployments, explosive manufacturing, and clandestine drug labs can be achieved by using the atmospheric dispersion parameters of their emitted chemical effluent streams. A chemical sensor downwind from a suspected emission point quantifies the emission concentration. This analytical model unifies atmospheric dispersion and other meteorological phenomenon of chemical interests with a developed mobile mass spectrometer system. As mobile mass spectrometer and other chemical sensors are developed, applying a reverse atmospheric model to datasets will provide an additional avenue to determine how sources of clandestine drug manufacturing, CWA deployment, and explosives manufacturing produce effluent stream behavior. This will lead to better Earth-Based Separation models, allowing real-time chemical separation; aiding in the minimization and prevention of chemical exposure while determining the source location of the emission itself.

Evaluation of Portable Linear Ion Trap Mass Spectrometer Coupled to Paper Spray Ionization Source for the Detection of Chemical Warfare Agents

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In spite of over a century of efforts to eradicate chemical weapon stockpiles around the globe, these compounds continue to pose a serious threat to military and civilian populations. The detection and identification of chemical warfare agents (CWA) in the field is currently dominated by portable ion mobility spectrometry (IMS), but is also performed with colorimetric and portable mass spectrometry (MS) systems. However, IMS and colorimetric systems often suffer from high false positive rates, poor resolution, high limits of detection, and detector saturation. Portable MS represents the best overall combination of size, accuracy, and ruggedness. In addition, ambient ionization techniques such as DART, paper spray (PS), and others represent a simplified approach to sample introduction, often requiring little to no sample preparation for samples taken directly in the field. In order to assess the ability of a portable mass spectrometer to reliably detect CWA chemistries utilizing a paper spray ionization source, dilute samples of the G-series and V-series of CWA were analyzed using this PS technique with a Bayspec Portability linear ion trap mass spectrometer. CWA was introduced onto a paper spray ticket along with spray solvent, and the system evaluated for limits of detection, reliability, and speed of analysis. This portable system showed limits of detection suitable to field analysis, and the ease of sample introduction along with the light weight (~17 lbs) of the instrument showcase its ability to reliably detect minute quantities of CWA in battlefield environments.

A Quadrupole Ion Trap for the Detection of Biomarkers at Icy Worlds

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A quadrupole ion trap (QIT) mass spectrometer (MS) has been designed and built for the detection of biomarkers on icy worlds. The presence of icy plumes in the solar system like those found at Saturn's moon, Enceladus, has sparked interest due to their potential to contain signs of life. In the case of Enceladus, a subsurface ocean is responsible for feeding cryovolcanoes, which eject small ice particles several kilometers away from the surface of the moon's icy shell. Cassini demonstrated how a spacecraft travelling several km/s can easily sample these plumes and obtain mass spectra during a flyby. However, Cassini's instruments did not have the ability to identify potential biomarkers. We have made modifications to the Spacecraft Atmosphere Monitor (SAM) QIT-MS, making it possible to sample ice grains at hypervelocities and detect the biomarkers they contain.

A notch was cut into one of the end caps of the QIT-MS to allow ice grains to enter the trapping region and impact the ring electrode. Upon collision of an ice particle with the ring electrode at hypervelocities, its constituents will be volatilized and/or ionized. In the lab, volatilization of aqueous biomarker solutions inside the QIT-MS was achieved by flowing solutions of fatty and/or amino acids directly through an end cap and to the heated ring electrode. Volatilized material was then ionized via chemical ionization (CI). Water was used in combination with other CI gases in order to find a suitable CI gas mixture capable of softly ionizing various fatty and amino acids. The use of water vapor as a collision gas for tandem MS was also demonstrated. Future plans of coupling the modified QIT-MS to a hypervelocity ice gun to better simulate ice plume sampling during a spacecraft flyby will also be discussed.

Optimization of a drone based miniature mass spectrometer system (Drone-MS) for in situ gas plume measurements

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In the 2017 HEMS workshop, we presented the results of the first flight testing of a miniature mass spectrometer prototype system integrated to an octocopter drone flown over Solfatara Volcano, Italy to demonstrate the capabilities of an autonomous airborne system for measuring volcanic gas emissions.

The 8 kg Drone-MS prototype included a modified XPR3 miniature quadrupole mass spectrometer from Inficon Inc. (1-100amu, 10^{-3} torr range operating pressure), together with a miniature turbo pump (either from CREARE LLC or Pfeiffer Inc.) two diaphragm pumps (rough pump and sample bypass), an embedded PC, a Lipo battery and telemetry integrated to an ITALDRONE octocopter with 10kg payload capabilities, 1km range and 20 min of endurance. Since the publication of the first results, there has been an increasing interest from researchers, volcanic observatories and other in situ surveying companies for introducing drones and unmanned aerial vehicles (UAV) with gas sensing capabilities for routine in situ gas monitoring in different applications.

The prototype flight testing was successful but showed areas of optimization needed to provide a ready to fly UAV-MS system to conduct routine in-situ gas measurements and 3D area surveys. Therefore, the original Drone-MS system has been progressively modified to decrease its weight by 25%, improve the vacuum system, fine tune the miniature quadrupole mass spectrometer's parameters to the target gases, and increase its endurance to drone vibration and high turns. The talk covers most of the optimizations to make the system flight ready for an Etna Volcano deployment scheduled for late October 2018.

The long term goal is to develop UAV payloads to conduct systematic in-situ measurements in a variety of applications, for example calibration and validation of remote sensing data using volcanic plume measurements, characterization of volcanic emissions and determination of chemical composition ratios that are used as precursor to bigger eruptions without the need of risking human lives, oil/gas pipe and landfill or chemical exposed area surveys and other application that requires systematic unmanned in-situ airborne measurements.

TRAVEL TIPS

DON'T FORGET YOUR POWER PLUG ADAPTERS!



If traveling by train in Germany the DB Navigator app is very useful. You can link a credit card and buy tickets after you find a spot on the train. I fly into Frankfurt and take a 1 hour train ride to Cologne. This is often much faster than trying to fly directly to Cologne from the USA.

THINGS TO DO IN COLOGNE:



If you have some free time to explore, Cologne is a beautiful city. Exploring the cathedral (DOM) is a must. You can climb the tower for spectacular views of the city (500+ steps, entrance down the stairs to the right when facing the front). You can also visit the museum (entrance on the side facing the train station) where you can see relics from the Three Wise Men which were apparently gifted (cough, cough) from an Italian church centuries ago and many other interesting artifacts. You probably won't need a map to find it.



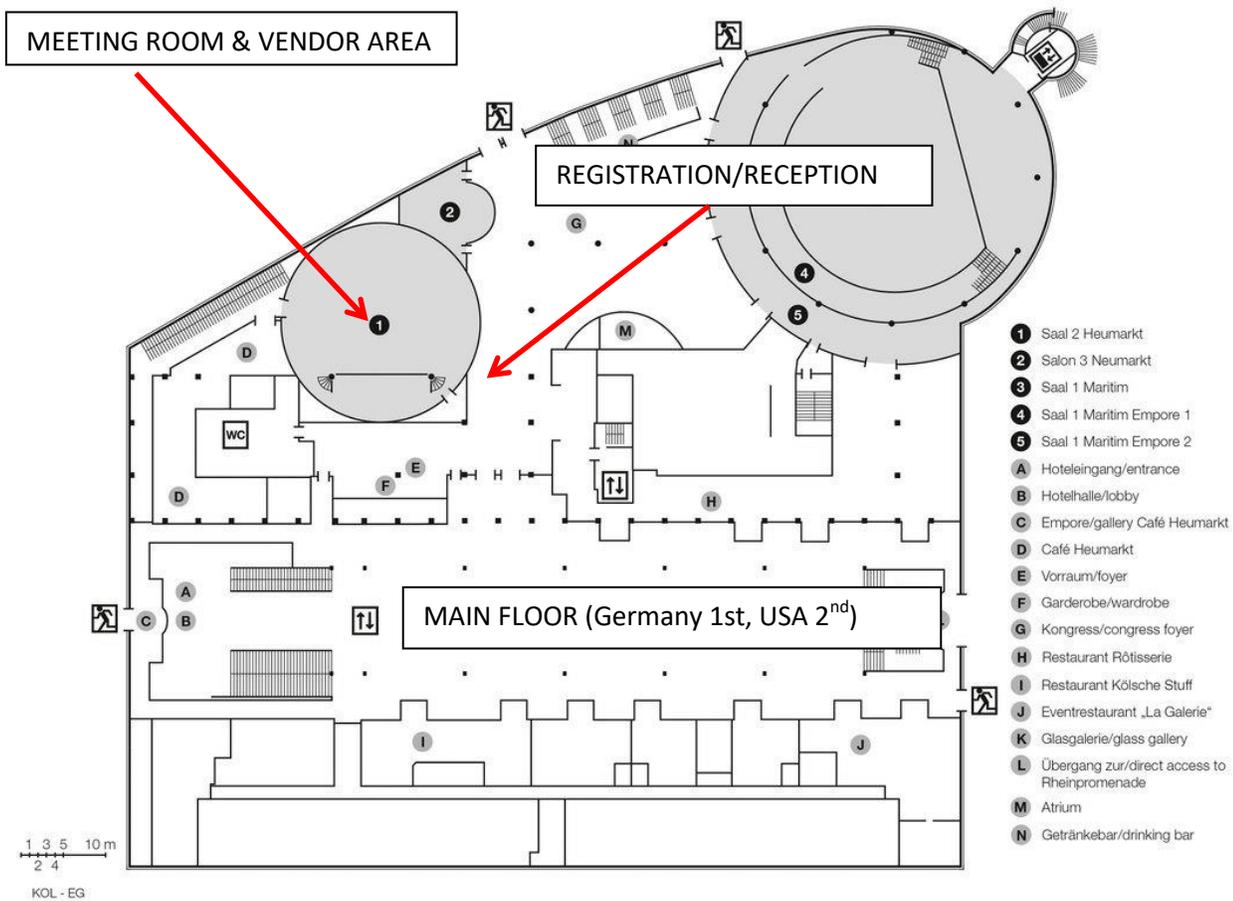
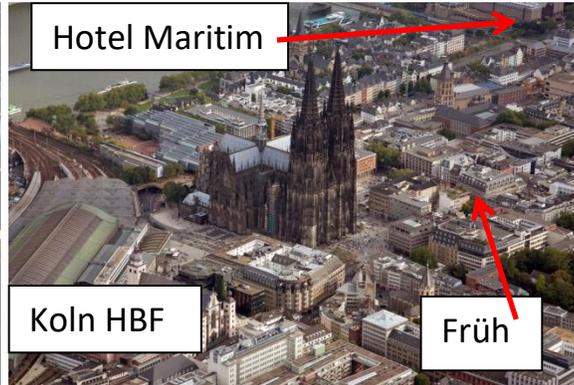
Chocolate Museum (www.schokoladenmuseum.de/en/). You'll want to save some room in your luggage. It's a 10 min walk along the Rhine from the hotel.

Riverboat tours can be fun and there are many other museums and interesting sights. The local beer is called Kolsch and it's quite good if you want to visit the some of brauhaus' in the old city. While it's all the same style there is still a lot of variation. My personal favorite is Fruh followed by Reissdorf, Malzmuhle and Paffgen. If you visit Brauhaus Sion to help them celebrate their 700th year of operation be sure to get the apple strudel - it's the best in the city. Weinhaus Brungs has the best traditional flammkuchen....so many good spots!

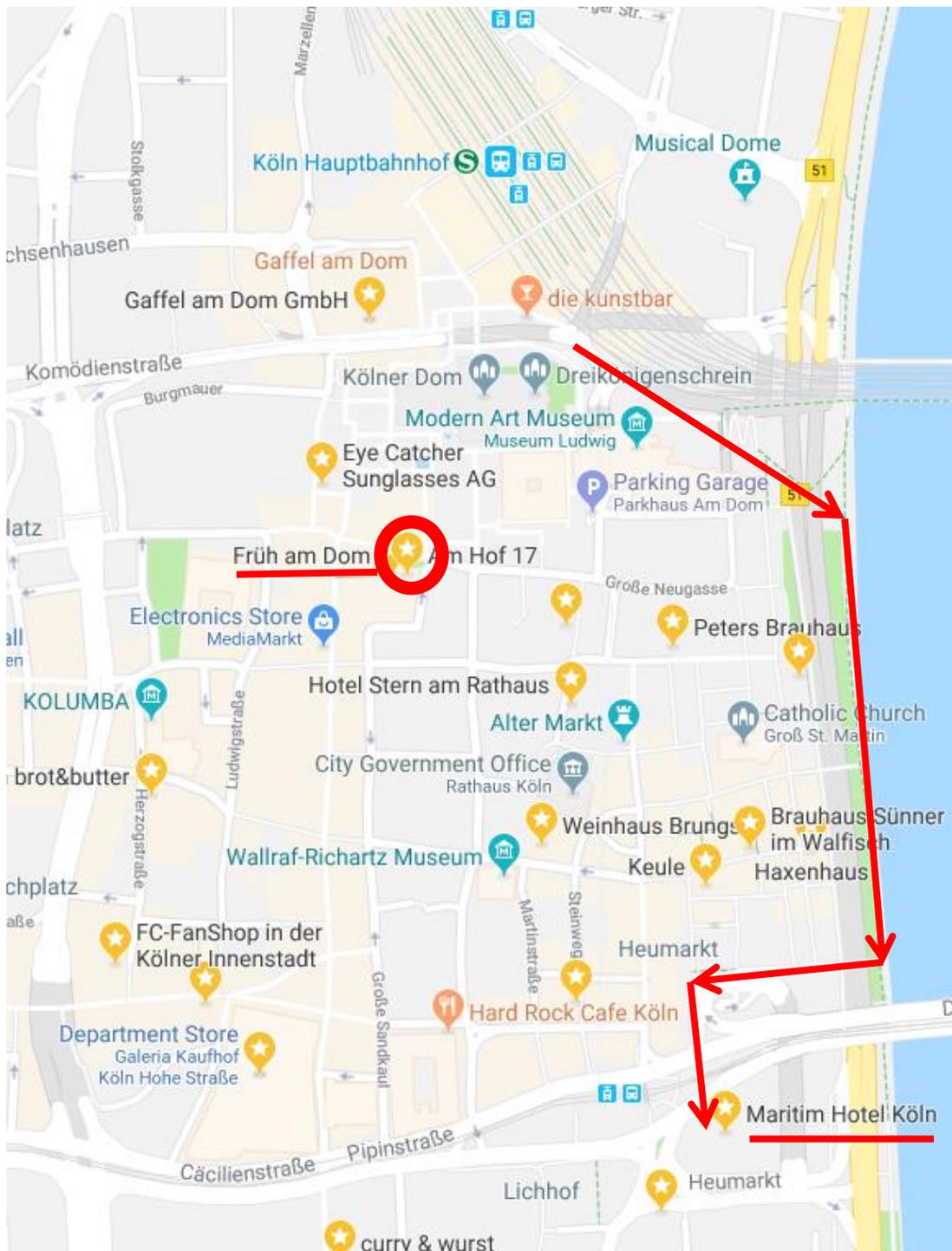
HOTEL AND MEETING ROOM

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EVERYONE HAS GOOGLE BUT...



If you want to walk with your luggage from the train station I recommend walking along the Rhine. It will be a much smoother ride for your luggage compared to the cobblestones of the old city!