Fourth Progress Report of the Joint Mass Spectrometry Centre of the University of Rostock and the Helmholtz Zentrum München and Initial Report of the Helmholtz Virtual Institute of Complex Molecular Systems in Environmental Health: Aerosols and Health (HICE)

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I am very happy to present the fourth progress report of the Joint Mass Spectrometry Centre (JMSC). The JMSC is a joint facility of the Helmholtz Zentrum München (Comprehensive Molecular Analytics, CMA) and the University of Rostock (Institute of Chemistry, Chair of Analytical Chemistry), focusing on the development and application of mass spectrometric and chromatographic methods for molecular analysis of complex systems in environmental science, health research and industrial research and development.

The past academic year was characterised by two important events. Firstly, in summer 2011 the Munich part of the JMSC (CMA), with its particular focus on aerosol research, was evaluated by an international review panel at the Helmholtz Zentrum München (HMGU). The review (mid-term evaluation) of the HMGU was conducted in the framework of the quinquennial cycle of the program-oriented funding scheme (POF) of the Helmholtz Association (HGF). The CMA successfully passed the evaluation with the best possible marks, which of course is an acknowledgement and huge motivation for all CMA co-workers.

The second particularly momentous event in the reporting period is the successful application for a Virtual Helmholtz Institute (VHI). One of the objectives of VHI’s is to strengthen the cooperation between Helmholtz centres and universities. They are funded by the HGF, once selected in a very competitive application procedure. In the funded Helmholtz Virtual Institute of Complex Molecular Systems in Environmental Health - Aerosols and Health (HICE) the cooperation between the Helmholtz Zentrum München and the University of Rostock is further strengthened. Moreover, several national as well as international and associated partners participate in HICE. HICE started operation on 1 January 2012. I need here to extend thanks to the Rector of the University of Rostock, Prof. Dr. Scharek, and the CEO of the HMGU, Prof. Dr. Wess, for covering the required co-payment of the University of Rostock and the HMGU. In the present annual report a presentation of HICE and the additional HICE partners is thus provided as well. Finally, I would like to thank the co-workers and the supporters of JMSC and HICE again and hope that the following academic year will be as successful as the preceding one.

Prof. Dr. Ralf Zimmermann
Head of the JMSC
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Concept of the Joint Mass Spectrometry Centre
Concept of the Joint Mass Spectrometry Centre (JMSC) of the University of Rostock and Helmholtz Zentrum München

Since April 2008, the University of Rostock (Chair of Analytical Chemistry) and the Helmholtz Zentrum München (CMA) have been cooperating in the field of development and application of mass spectrometry-based analytical techniques for the characterization of complex molecular substance mixtures.

For this purpose, a cooperation contract between the University of Rostock and the Helmholtz Zentrum München was signed, creating the “Joint Mass Spectrometry Centre” (JMSC) as a joint research activity. The JMSC is headed by Prof. Dr. Ralf Zimmermann, who concurrently holds the Chair of Analytical Chemistry at the University of Rostock (UR) and directs the cooperation group at Helmholtz Zentrum München (HMGU). This cooperation group had been restructured in March 2011 to form the independent cooperation group “Comprehensive Molecular Analytics” (CMA). The JMSC is thus formed by the CMA and the Chair of Analytical Chemistry (CAC) of the University of Rostock. At the University of Rostock, the Joint Mass Spectrometry Centre (JMSC) is represented by the Chair of Analytical Chemistry. It is located in the buildings of the University of Rostock at Dr.-Lorenz-Weg. Currently 17 academic staff members (senior scientists, postdocs, PhD students and diploma students) are employed at the Chair of Analytical Chemistry. Three members occupy permanent academic positions, while nine members have temporary third-party funded employment contracts. There are also three scholarship holders. Facilities in Rostock comprise 515 m² of laboratory space (200 m² for teaching) and 125 m² of office space, including an office container.

JMSC Research Areas

Research topics of the JMSC are structured in three research areas with corresponding research groups at UR and HMGU (Figure 1).

The objective of the first research area of the JMSC is to study environmental aspects and their impact on human health. The main objective of the research group “Environmental and Process Analysis” in Rostock is the analysis of chemical signatures of significant technical and environmental processes. The corresponding group at the HMGU is “Health Relevant Environmental Analysis – Aerosol Research” (HAR). It is embedded in the framework of the HMGU “Environmental Health” POF program and focuses its research activities on ambient aerosols and their health effects.

The second research area of the JMSC is concerned with biomedical and health-related applications. One focus of the unit “Biomedical Analysis” in Rostock is the comprehensive analysis of breath gas which is performed in cooperation with the Rostock University Hospital. The corresponding research area in Munich is named “Comprehensive Molecular Profiling” (CMP). It develops and applies novel multidimensional profiling techniques for non-targeted metabolic characterisation, for instance in diabetes.
On 2 July 2009, the public inauguration of the Joint Mass Spectrometry Centre took place in the historical main building of the University of Rostock.

Image 1 | Campus of Helmholtz Zentrum München.

Image 2 | University of Rostock. On 2 July 2009, the public inauguration of the Joint Mass Spectrometry Centre took place in the historical main building of the University of Rostock. Image source: ITMZ/University of Rostock.
research or in cell-based toxicological studies on the effect of inhaled aerosols. The third research area of the JMSC is “Analytical Method Development” (AMD). It is identically named at both institutions. In Rostock, the AMD focuses on the advancement and implementation of single and multiphoton ionisation technologies. The photon sources consist of laser or lamp-based light sources, such as electron-beam pumped rare-gas excimer light sources (EBEL). At the HMGU, research is concerned with the development and application of joint analytical systems. Examples include comprehensive two-dimensional gas chromatography and thermogravimetry (TG) coupled to single-photon ionisation time-of-flight mass spectrometry.

**Facilities and Equipment**

At the University of Rostock, the Joint Mass Spectrometry Centre (JMSC) is represented by the Chair of Analytical Chemistry. It is located in the buildings of the University of Rostock at Dr.-Lorenz-Weg. Currently 17 academic staff members (senior scientists, postdocs, PhD students and diploma students) are employed at the Chair of Analytical Chemistry. Three members occupy permanent academic positions, while nine members have temporary third-party funded employment contracts. There are also three scholarship holders. Facilities in Rostock comprise 515 m² of laboratory space (200 m² for teaching) and 125 m² of office space, including an office container. Research equipment and instrumentation in Rostock include six photoionisation-

![Organisational chart of the Joint Mass Spectrometry Centre (JMSC).](image)

**Figure 1 | Organisational chart of the Joint Mass Spectrometry Centre (JMSC).** The JMSC is divided into three corresponding research areas at the University of Rostock and the Helmholtz Zentrum München. They intensely cooperate with each other. The cooperation partner bifa Environmental Institute GmbH and Photonion GmbH are closely related to research areas 1 and 3, respectively.
time-of-flight-mass spectrometers and one proton transfer mass spectrometer for online analyses (breath gas analysis, combustion and pyrolysis analysis, process analysis). A laser laboratory is available for the application and development of photoionisation techniques (Nd:YAG laser, tunable OPO and dye laser, CO2 laser, excimer laser, electron-beam pumped rare-gas excimer light sources), two LC-MS systems and several GC-MS used for method development. For applications of analytical pyrolysis, combustion research and pyrolysis research, a pyrolysis furnace with two chambers and a pyrolyzer that is interconnectable with a GC/MS are available. For development and application in thermal analysis, a thermo balance system, coupled by a skimmer-molecular beam-interface to a quadrupole mass spectrometer system is available. Thermodesorption equipment is available to study carbon content in solid samples. It is coupled to a photo ionisation mass spectrometer. Finally, a laboratory reactor used to study Fischer-Tropsch synthesis (heterogeneous catalysis) was implemented.

In addition, the research group of PD Dr. Gerd-Uwe Flechsig, conducting research in electrochemical analytics, is located at the Chair of Analytical Chemistry. It currently consists of three PhD students.

The cooperation group “Comprehensive Molecular Analytics” (CMA) at Helmholtz Zentrum München in Neuherberg consists of 25 scientists. Thirteen scientists are permanently employed at Helmholtz Zentrum München. Two are exempt employees, working as Helmholtz employee representatives for half a day. 10 PhD students are employed on a temporary basis with contracts through third-party funding. The cooperation group also has four technical staff members and two retired scientists serving as associated scientific consultants.

The cooperation group in Neuherberg operates two HPLC-MS/MS systems, two HPLC systems equipped with a diode array and fluorescence detector, one system for multi-dimensional gas chromatography-time-of-flight mass spectrometry (GCxGC-TOFMS), four GC-MS systems (one TOF, three for thermo desorption) and several instruments coupled for thermal analysis (TG, DSC, etc.) with EI-quadrupole mass spectrometry and FTIR. Physicochemical characterisation of particulate matter and aerosol particles is performed using a high resolution aerosol mass spectrometer (AMS, WTOF), a particle sizing instrument (a scanning mobility particle sizer (SMPS)), two electric low pressure impactors (ELPI), an aerodynamic particle sizer (APS), a white light optical particle sizer (WELAS)
and particle sampling equipment (several Berner impactors, a rotating-drum impactor, a MOUDI impactor and several low volume samplers).

In the framework of the current activities in the field of analytical method development we use and are currently implementing the following, rather experimental instruments:

- A laser desorption/thermodesorption - resonance enhanced multiphoton ionisation - single particle - time of flight mass spectrometer (LD-TD-REMPI-SP-TOFMS) for the online characterisation of aerosol particles;

- A laser-desorption ionisation / laser-desorption resonance enhanced - multiphoton ionisation / single-photon ionization - time of flight mass spectrometer (LDI/LD-REMPI/SPI-TOFMS) for the analysis of solid samples, sampled aerosol particles and biological samples;

- A thermal analysis - single-photon ionisation - quadrupole mass spectrometer (TA-SPIxMS);

- A thermal analysis - single-photon ionisation - time of flight mass spectrometer (TA-SPI-TOFMS) for the determination of organic signatures in thermal processes.

Three instruments for the multi-dimensional analysis of highly complex samples in bioscience and environmental science are available in the group:

- Thermal analysis - single-photon ionisation comprehensively coupled with gas chromatography time of flight mass spectrometry (TA-GCxSPI-TOFMS);

- Gas chromatography - EBEL-single-photon ionisation - time of flight mass spectrometry (GCxSPI-TOFMS);

- Comprehensive two-dimensional gas chromatography - EBEL-single-photon ionisation - time of flight mass spectrometry (GCxGC-TOFMS) including two thermodesorption - photo ionisation - ion trap - mass spectrometers (TD-SPI-ITMS) for the determination of security-relevant compounds (drugs, explosive substances and etc.).

Research Facilities

Members of the Munich branch of the JMSC are currently dispersed in several buildings on the campus of the Helmholtz Zentrum München (bldg. 16, 24, 38c and 57), but reconstruction and renovation work in building 24 is being carried out. The renovated building will bring together all members of the research group in the near future.

In Rostock, the research building of the Department Life, Light and Matter (LLM) is under construction at the Rostock University „Südstadt“ Campus.

Image 5 | View of the construction site LLM (Department Life, Light and Matter) at „Südstadt“ Campus of the University of Rostock.

From 2015 the JMSC will operate a mass spectrometry facility for special applications in the research building. Furthermore, the erection of the plant extension building of the Institute of Chemistry will start in 2014.
Hence due to the new buildings and the current reconstruction work in the Neuherberg part of the JMSC, we expect high-end research facilities for the whole JMSC in the near future both in Munich and in Rostock.

The bifa Environmental Institute: Cooperation and Projects

The Joint Mass Spectrometry Centre cooperates with the bifa Environmental Institute through a contractual partnership with the CMA. The bifa is a non-profit limited liability company (GmbH) with the State of Bavaria, the Chamber of Industry and Commerce of Swabia and the City of Augsburg as shareholders. It is an application-oriented scientific institute located in Augsburg and provides a supply of services in development, engineering and consulting focused on technical environmental protection for its customers. Prof. Dr. Ralf Zimmermann has served as external director of the subject area “chemistry” at the bifa. One employee of the bifa currently works as senior scientist in a third-party funded project of the JMCS on the fundamentals of work place aerosol characterisation.

Technology Transfer: Photonion GmbH

Ongoing developments in online single-photon ionisation mass spectrometry (SPI-MS) in our cooperation group have led to a number of patents and third party projects, often carried out with direct industrial support.

To satisfy the upcoming demand, a spin-off company was founded: Photonion GmbH. It is closely connected to scientific research and aims at the further development of innovative trace gas analysis instruments based on the single photon ionisation-mass spectrometry (SPI-MS) techniques and expertise of the JMSC.

The SPI-MS technique involves an electron-beam pumped excimer light source (EBEL), which allows the efficient and soft ionisation of organic compounds. SPI-MS is applicable for on-line analysis of complex mixtures of organic compounds. Various applications, for instance in process and product surveillance for food, drugs, mineral oil, chemical and medical products have been performed. The technique is also used in fundamental and applied research, for example for the analysis of synthetic material, the quality assurance of petrochemical feedstock and natural products and also for the
analysis of thermal processes, such as the puff-resolved analysis of pollutants in tobacco smoke. Partners of Photonion GmbH are Ascenion GmbH (patent realisation association of the Helmholtz Zentrum München), Tofwerk AG (custom time-of-flight mass spectrometers in Thun, Switzerland) and Airsense Analytics (innovative sensor technologies and safety equipment in Schwerin, Germany).

Seed capital came from these partners and from a presidential grant (HEF) of the Helmholtz Community (HGF). Research-related parts of Photonion are located at Helmholtz Zentrum München. The head office is based at Airsense Analytics, Schwerin.

Image 8 | Main building of Photonion GmbH.
News and Highlights
News and Highlights of Summer Term 2011 and Winter Term 2012 - Progress Overview

In the third year of its existence, the Joint Mass Spectrometry Centre succeeded in the development of further instrumental methods applicable for a wide variety of analytical issues.

As mentioned, the Cooperation Group at the Helmholtz Zentrum München was renamed in “Comprehensive Molecular Analytics” (CMA) and became independent from the “Institute of Ecological Chemistry,” which finally was closed at the end of 2011.

Foundation of HICE

The reporting period was dominated by the preparation and defense of the proposal to found HICE, i.e. the „Helmholtz Virtual Institute of Complex Molecular Systems in Environmental Health: Aerosols and Health“. The funding period started on January 1, 2012. Under the general management of Prof. Zimmermann, the health effects of anthropogenic aerosols shall be studied during the funding period.

Besides the JMSC and the partners from Helmholtz Zentrum München [the Comprehensive Pneumology Center / Institute of Lung Biology and Disease, the Institute of Biomathematics and Biometry, and the Research Unit Medical Radiation Physics and Diagnostics] and from the University of Rostock (the Department of Piston Engines and Internal Combustion Engines, the Department of Systems Biology and Bioinformatics, and the Institute of Physics) the following national and international partners cooperate in HICE:

May 6-7, 2011
3rd Sino-German Workshop on Air Quality and Health Research, Beijing, China.

May 8, 2011
Visit of Lanzhou University in Gansu Province and its observation stations.

May 16-20, 2011
Installation of Bruker FTICR-MS at the laboratory in Rostock.

May 23, 2011
Operation of Bruker FTICR-MS begins.
• Karlsruhe Institute of Technology;
• Max Delbrück Center for Molecular Medicine Berlin-Buch;
• Technische Universität München;
• University of Cardiff;
• University of Luxembourg;
• University of Eastern Finland.

A number of further partners are associated to HICE, including ASG Analytik-Gesellschaft, Vitrocell Systems GmbH, Decodon GmbH, Photonion GmbH, and the JRC and Sustainable Transport Unit (STU) - VELA Laboratory.

The Pre-Kickoff Meeting of HICE was held from November 10-11, 2011 in Neuherberg at the Helmholtz Zentrum München (HMGU). The subsequent meetings of work packages III and IV were held on December 16, 2011 also at the HMGU and of work packages I and II on February 6, 2012 at KIT in Karlsruhe.

**Bruker FTICR-MS Installed**

In May 2011 the new Bruker Fourier transform ion cyclotron resonance mass spectrometer was installed at the laboratory in Rostock and started its operation on May 23, 2011.

This instrument, which will be used by a number of cooperating working groups, will establish new possibilities for the characterisation of complex mixtures (e.g. mineral oil, pyrolysis products, soil constituents, drugs and metabolites) due to its ultra-high mass resolution. The modular set up of the inlet system allows the direct coupling of a GC and the gas inlet of already established pyrolysis and thermogravimetry experiments.

**Conference Participation**

In the beginning of May 2011, the 3rd Sino-German Workshop on Air Quality and Health Research was held in Beijing, Peoples Republic of China. The major goal of this workshop was to support and intensify existing collaborations in the field of urban atmospheric pollution and health between Chinese and German scientists and to initiate new interactions. The workshop was completed by a visit of Lanzhou University in Gansu Province and its observation stations.

In June 2011, a joint PM2.5 measuring campaign started in Beijing and...
Xianghe in Hebei Province, east of Beijing, simultaneously.

The Cooperation Group was represented at the 10th International Conference on Carbonaceous Particles in the Atmosphere (ICCPA) in Vienna, Austria, from June 26-29, by a presentation on characterization of wood combustion sources.

The autumn conference season started with the workshop “Aerosols from domestic biomass heating – characterization and toxicity” in Manchester at the beginning of September and went on with the European Aerosol Conference from September 4-9, 2011 in Manchester, too. In the beginning of October, the Aerodyne AMS Users’ Meeting took place in Orlando, Florida, preceding the American Association for Aerosol Research Conference (AAAR) 2011 at the same place.

Scientific Exchange

At the beginning of November 2011 at the Leibniz Institute for Baltic Sea Research in Warnemünde a lab with a new NanoSIMS (nano secondary ion mass spectrometer) was opened, which is applied for sensitive analysis of solids in cooperation with the JMSC. Analytical NanoSIMS imaging is perfectly suited to measure, visualize and quantify the distribution of elements and their stable isotopes in environmental samples or at the sub-cellular level in biological material. Following the opening, the European User Meeting for these rare instruments was held at the same place. In January 2012 a group of students of the Rostock branch of the JMSC made an excursion to Thermo Fisher Scientific in Bremen to be informed at firsthand about the development of new analytical instrumentation. The scientific exchange was additionally intensified by several visits of Ralf Zimmermann to the United States, China, Zurich, Grenoble and Bruges as well as by a number of visits of scientists and company representatives in Rostock and Neuherberg.

Completed PhD Theses

During the reporting period, two PhD students completed their dissertation theses. Sebastian Dresen defended his thesis on July 5, 2011, on the topic “Entwicklung neuer LC-MS/MS Methoden und deren Anwendung in der Forensischen Toxikologie.” For this dissertation a liquid chromatography-tandem mass spectrometry (LC-MS/MS) library of mass spectra of over 1250 compounds relevant in clinical and forensic toxicology was...
created using a hybrid mass spectrometer (triple quadrupole with linear ion trap). These mass spectra can be used for the identification of compounds in biological matrices and also for the development of LC-MS/MS methods to detect those compounds by monitoring specific fragments after selecting their corresponding molecular ions.

Both possibilities were used to create a multi-target screening which can be used complementary to established gas chromatography-mass spectrometry (GC/MS) and high performance liquid chromatography-diode array detection (HPLC-DAD) screening methods used in routine analysis. Furthermore, a screening method for the detection of new designer drugs was developed. LC-MS/MS methods for the quantitation of certain compound classes (basic drugs, cardiovascular drugs) in serum were developed and validated following international guidelines. This was also performed for synthetic cannabinoids which were identified as additives in herbal mixtures being not part of routine screening methods.

On July 12, 2011, Markus Eschner successfully defended his thesis on the topic “Coupling of Gas Chromatographic Methods with Single Photon Ionization Mass Spectrometry for Multidimensional Characterization of Complex Samples.” This work describes the realization of novel concepts in coupling of gas chromatography (GC) to mass spectrometry (MS) by utilization of soft single photon ionization (SPI) on the basis of the electron-beam pumped rare gas excimer light source (EBEL).

The innovative EBEL technique enables generation of intense and brilliant vacuum ultraviolet (VUV) radiation. By means of SPI-MS molecules can be detected mostly fragmentation-free. Thus, molecules with different molecular ion masses can be separated within the same mass spectrum resembling a boiling point separation in GC. Furthermore, by combining GC and SPI-MS a comprehensive two-dimensional characterization (GC×MS) of complex samples can be obtained which is in its results similar to comprehensive two-dimensional gas chromatography (GC×GC).
Mid-Term Evaluation

At the end of June and the beginning of July 2011 the scientific performance of the cooperation group in Neuherberg (CMA) was evaluated by an international review panel in the course of the mid-term review of the program oriented funding scheme (POF II) of the Helmholtz Association (HGF).

The CMA eventually passed the evaluation with the best possible marks, which of course is an acknowledgement and huge motivation for all CMA coworkers.

During the reporting period, the scientist Dr. Konstantinos Oynos retired.

The annual joint seminar of the JMSC was held in Rostock at the end of July that year. Besides the intensive scientific exchange social activities didn’t miss out, the weather was fine and there were no mountains to climb. Instead, we arranged an excursion to Prerow and the genuine landscape of the Darss, which is part of the national park “Vorpommersche Boddenlandschaft.”
New Phd Students
Michael Fischer  
**Helmholtz Zentrum München**  

In September 2010, Michael Fischer successfully completed his Diploma in Geoecology in Bayreuth. After working one year for Siemens in the field of industrial environmental protection, he joined the CMA and started his PhD in October 2011.

His work focuses on instrument development and optimisation of a new technology for fast multidimensional chemical analysis of thermal processes, with a special focus on good science applications. The doctorate is embedded in a joint research project between NETZSCH Gerätebau GmbH, Photonion GmbH and the CMA group, and is funded by the Bavarian Science Foundation (BFS).

The objective of his research is to build up a performing, scientific, well evaluated demonstrator device based on Thermal Analysis (TA), fast gas chromatographic methods (fast-GC) and time-of-flight mass spectrometry (ToF-MS) using rapid Electron Impact ionization/single-photon ionization (EI/SPI) switching. Michael collaborates with Sebastian Wohlfahrt, who also is involved in the BFS project.

Beate Gruber  
**Helmholtz Zentrum München**

Beate Gruber studied Food Chemistry at Dresden University of Technology and received her diploma in 2010.

Two different analytical aspects are in the scope of her thesis with the subject “Determination of Relevant Substances in Biological Samples.” As a first part of her work, methods for the bio-monitoring of polycyclic aromatic hydrocarbons (PAHs) and PAH metabolites in blood (sample volume 1 µl) and urine are developed. The second part deals with the comprehensive molecular analysis of breath gas (BGA) as a non-invasive metabolic monitor for the diagnosis and development of individualised preventive strategies for type 2 diabetes (postpartum) in mothers and their offspring.

The aim is the identification of a preferably small group of relevant volatile organic compounds (VOCs) in breath gas using comprehensive two-dimensional gas chromatography. This should allow the separation of individuals who will postpartum develop impaired fasting glucose (IFG), impaired glucose tolerance (IGT) and type 2 diabetes in the mothers and offspring from healthy individuals.
Kornelia Lau  
*University of Rostock*

Kornelia Lau studied Chemistry at the University of Rostock and received her diploma at the Leibniz-Institute for Catalysis in September 2011. Her research is on „Fuel and biofuel transformations and their deposits.” The aim of this study is to characterise the main compounds which cause deposits in diesel engines and to understand their formation mechanism. These compounds are analysed by chromatographic and mass-spectrometric methods, like GC-MS, Pyrolysis-GC-MS, TA-(GCx)-SPI-MS and GCxGC-MS. The work is carried out in cooperation with the Faculty of Mechanical Engineering and Ship Building at the University of Rostock.

Fengxia Li  
*Helmholtz Zentrum München*

Fengxia Li studied Environmental Health at Peking University, School of Public Health. She received her Master’s degree in 2011. In 2011 she successfully applied for a PhD scholarship from the Chinese Scholarship Council (CSC). The subject of her PhD work is “Development and application of analytical methods for quantification of oxidized organic aerosol components in ambient particulate matter.”

The major objectives of her research are to identify and quantify relevant constituents of PM, to differentiate the sources of secondary (SOA) and primary (POA) organic aerosols, to identify the main sources of ambient PM and to determine mechanisms for “high” PM load in the greater Beijing area. PM2.5 samples collected in cooperation with the Institute of Atmospheric Physics, Chinese Academy of Science, will be analysed for chemical composition. Special attention is paid to the development and validation of a GCxGC-MS based method for the quantification of oxidized compounds in PM samples.
Christian Radischat
University of Rostock

Christian Radischat studied chemistry and received his diploma at the University of Rostock in September 2011. The topic of his doctorate is the “On-line combustion analysis of biomass and biofuels”. The aim of this study is to quantify organic compounds in emissions from combustion sources, which are potentially responsible for adverse health effects. Therefore his research is part of the HICE Virtual Institute.

On-line and real-time techniques for the determination of the gaseous organic combustion products are further developed and applied. The studies include the emissions from diesel and biofuel powered vehicles and the exhausts from the combustion of biomass. For a selective and sensitive detection of aromatic compounds a multiphoton ionisation source based on UV laser pulses ($\lambda = 266$ nm) is used. The single photon ionisation technique ($\lambda = 118$ nm) is used for the detection of aliphatic compounds. In the HICE project, Christian Radischat’s work partly overlaps with that of Ahmed Reda, who is responsible for the off-line quantification of reactive gas phase species.

Ahmed Reda
Helmholtz Zentrum München

Ahmed Abd Alhadi Reda studied Analytical Chemistry at Al Nahrain University, Iraq and received his Master degree in science in 2004. Since then he had worked as lecturer and instrumental specialist at Al Nahrain University and the Iraqi Ministry of Science and Technology. In 2010 he successfully applied for a scholarship from the German Academic Exchange Council (DAAD) He joined the CMA in October 2011.

His doctorate is focused on the „Development and application of methods for sampling and characterisation of volatile organic compounds in emission aerosols“. He attempts to identify and quantify reactive (semi) volatile organic compounds (S)VOCs in emission aerosol in terms of oxygen content. One focus of his work will be the development of GCxGC-MS based methods for the comprehensive characterisation of (S)VOCs samples from biofuel combustion. The work contributes to HICE. He is cooperationg with Christian Radischat, who is responsible for the on-line determination of gas phase species.
Aimée Celestè Sutherland  
Helmholtz Zentrum München

Aimée Celestè Sutherland completed her Master in Science, Chemistry and Polymer Science at the University of Stellenbosch, South Africa in 2010. After completing her studies she worked as a consultant for a Water and Environmental Engineering company (Emanti Management (Pty) Ltd in the business district of Stellenbosch.

In 2010 she received a scholarship from SASOL Technology (Pty) Ltd, South Africa. She officially joined the CMA group in January 2012. The main focus of her research is on the development and application of multidimensional comprehensive analysis methods for the investigation of chemical signatures in samples which are relevant for Fischer-Tropsch fuel synthesis. Classical GCxGC-TOFMS with Electron Ionization (EI) will be combined with LCxMS and photoionisation mass spectrometry approaches (SPI/REMPI). The latter technique will be used in a novel concept that should allow simultaneous detection of eluents by REMPI and EI (or SPI and EI). The use of chemometrics with these techniques will be investigated to improve our understanding of these streams.

Sebastian Wohlfahrt  
Helmholtz Zentrum München

Sebastian Wohlfahrt studied Chemistry at the Technische Universität München. He received his Master’s degree in Analytical and Organic Chemistry in 2011 and joined the CMA group in November 2011.

His work contributes to the joint research project “Fast multidimensional chemical analysis of thermal processes” between NETZSCH Gerätebau GmbH, Photonion GmbH and the CMA group, funded by the Bavarian Science Foundation (BFS, Bayerische Forschungsstiftung).

The main goal is to develop a new technology based on Thermal Analysis (TA), fast gas chromatographic methods (fast-GC) and Time-of-Flight mass spectrometry (ToF-MS) using Electron Impact and Single-Photon Ionization (EI, SPI). To achieve this aim, his work will include, among others, the construction of a suitable GC-modulator, the implementation of rapid EI/SPI-switching and the development of an integrated software solution. Michael Fischer contributes to this project, too.
New Research Projects
Comprehensive Molecular Analysis of Breath Gas

The project „Comprehensive molecular analysis of breath gas as a non-invasive metabolic monitor for the diagnosis and development of individualized preventive strategies for T2D (postpartum) in mothers and their offspring (combreath)” is a joint project between the CMA and the AMSD (Dr. Szymczak) in cooperation with the IDF 1 (Prof. Ziegler).

The study began in January 2012 and is focused on the investigation of the development of type 2 diabetes (T2D) in mothers and their offspring as a result of gestational diabetes mellitus (GDM). Due to the combination of non-invasive on-line proton transfer reaction mass spectrometry (PTRMS) and sensitive off-line gas chromatography for breath gas analysis (BGA), mechanisms and biomarkers for the differentiation of healthy and affected individuals are investigated. The objectives of the project are the identification of a preferably small group of VOCs in breath gas which allows the separation of individuals who will postpartum develop impaired fasting glucose (IFG), impaired glucose tolerance (IGT) and T2D in the mothers and offspring from healthy individuals, the identification of (preferably early) biomarkers and the recognition of metabolic pathways for the risk assessment to develop T2D and/or obesity postpartum of mothers and offspring, the establishment of a combined method for online and offline BGA sampling and to prove the feasibility of these combined techniques during an oral glucose tolerance test (oGTT) and a deeper understanding of dynamics and physiological mechanism of oGTT based on continuous metabolic online monitoring.

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Funding

The first year of the project is funded by the German Center for Diabetes Research in the field of translational and clinical projects (PhD student, consumables).

Web

www.helmholtz-muenchen.de/cma/ueber/mitglieder-der-arbeitsgruppe/index.html
In December 2011, a PhD project for the investigation of Fischer-Tropsch (FT) products and mechanisms of FT processes was launched at Helmholtz Zentrum München. The basis of the project is a Framework Research Services Agreement between Sasol Technology (Pty) Ltd and the University of Rostock.

While different FT products will be produced with a lab size FT reactor at the University of Rostock, the chemical analysis will be carried out in Munich. Chemical analysis is based on comprehensive two-dimensional gas chromatography (GCxGC), liquid chromatography x gas chromatography and high resolution mass spectrometry.

The combination of the different instrumentation with quantitative analysis and chemometric analysis of the data will give a comprehensive overview of the chemical signature of the FT product and the underlying processes.

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**Funding**  
The project is being funded by Sasol, Johannesburg, South Africa.

**Web**  
www.helmholtz-muenchen.de/cma/ueber/mitglieder-der-arbeitsgruppe/index.html

Figure 2 | GCxGC analysis of a FT product produced at the University of Rostock.
Diesel Exhaust Particles (DEP) are Involved in the Formation and Strengthening of Allergic Diseases

It is assumed that polycyclic aromatic hydrocarbons (PAHs) are responsible for the effects caused by DEP, regardless of the nature of the particles.

It is also assumed that the production of reactive organic species (ROS) induced by PAHs plays an important role (activation of NF-κB). Phenanthrene (Phe) is a main component of environmental PAHs and occurs in DEP. Since its metabolites are excreted in large amounts in the urine, Phe is of high diagnostic value in the biomonitoring of PAH exposure. Phe is a known substrate for cytochromes P450 (CYPs).

However, the multiple and overlapping specificities of CYPs cover the role of individual isoforms in PAH metabolism. In January 2012, a project based on two bachelor theses for the development of a new method for the determination of PAHs and their metabolites in human blood was started. The method will be based on the thermal extraction of the PAHs from a 1 µl blood sample, using a lancing device for capillary blood sampling and a 1 µl disposa capillary pipette. Whole blood elimination studies may help to elucidate the role of individual CYPs.

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Figure 3 | Sampling devices and analytical instrumentation.
New Technology for Fast Multidimensional Chemical Analysis of Thermal Processes

In October 2011, a joint project, funded by the Bavarian Research Foundation (Bayerische Forschungsstiftung), with the Netzsch Gerätebau GmbH and Photonion was started.

The objective of the project is the development of a Thermal Analysis (TA) instrument, coupled to fast-GC and Time-of-Flight mass spectrometry (ToF-MS). Special challenges are the search and adaption of a suitable modulator, the implementation of a rapid switching between electron ionisation (EI) and Single-Photon Ionization (SPI) as well as the provision of an integrated software solution. Passing further milestones, like the development of a High-Speed-STA-oven and the construction of a micro fast-GC-oven, the project will lead to the build-up of two performing demonstrator devices.

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Funding

This project is being funded by the Bavarian Research Foundation.

Web

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Figure 4 | Schematic setup of the TA-fast-GC-SPI/EI-ToF-MS.
Sustainable Use of Bioenergy: Bridging Climate Protection, Nature Conservation and Society

In February 2012, the second part of the project „Sustainable use of bioenergy: Bridging climate protection, nature conservation and society“ was launched.

The tapping of energetic potential from wood combustion is an important complementary source for bioenergy and is one of the topics of this interdisciplinary approach, founded by the Interdisciplinary Centre of Sustainable Development of the University of Göttingen. Question are: How can wood combustion contribute to a decentralized supply of energy when launching sustainable energetic concepts for a region? How large are the emissions which must be expected? Is it even possible to reduce the emissions by the construction of district heating networks in combination with local wood combustion plants? Therefore different kinds of wood combustion, different types of woods, and also alternative fuels like straw were investigated. Now the main focus is the study of the combustion properties of wood from short rotation coppice, both from non-contaminated and contaminated areas (e.g. soil absorption fields). The task of the CMA is to investigate organic emissions from wood combustion experiments and the assessment of the toxic potential of emitted particulate matter in cooperation with the University of Cardiff, UK. Further project partners are the Department of Sedimentology and Environmental Geology of the University Göttingen (inorganic characterization of PM) and the Technology and Support Centre in Straubing, Germany (operative accomplishments of combustion experiments).

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This work was supported by the Technology and Support Centre, Straubing, Germany, the Virtual Institute of Complex Molecular System in Environmental Health (HICE) and the Federal Ministry of Science and Culture, Lower Saxony, Germany.

**Web**

www.helmholtz-muenchen.de/cma/ueber/mitglieder-der-arbeitsgruppe/index.html

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**Figure 5** | Testbench at Technology and Support Centre (TFZ), Straubing (left). Combustion chamber of wood chip boiler (right).
Deposits Formed in the Injectors of Modern DI Diesel Engines

In January 2012, a joint project with the Chair of Piston Engines and Internal Combustion Engines of Rostock University was initiated.

The topic of this project is the investigation of deposits formed in the injectors of modern DI diesel engines. Thereby, a special emphasis is put on the content of biodiesel in the fuel. Artificial aging experiments of various diesel fuels and blends of diesel fuel with biodiesel are conducted, where the fuel is tempered for some days at a set temperature and the components of the fuel are analyzed before and after the tempering by means of gas chromatography/mass spectrometry. Selected samples are investigated more thoroughly by two-dimensional GCxGC. Furthermore, actual deposits on small injector parts generated in a common rail diesel injector test bench are analyzed by thermal desorption/pyrolysis with subsequent direct photo-ionisation mass spectrometry.

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Funding

The project is being funded by the „Fachagentur Nachwachsende Rohstoffe“ (FNR) and the „Forschungsvereinigung Verbrennungskraftmaschinen“ (FVV).

Web

www.chemie.uni-rostock.de/forschung/analytische-technische-chemie/dr-thorsten-streibel/

Figure 6 | Diesel engine injector part (A) in immaculate condition (B) after several days of engine operation.
Comprehensive Characterisation of Aerosol Gas-Phase and Particle-Phase from Wood Combustion Emissions

C. Busch (UR), M. Elsasser (HMGU/UR), J. Orasche (UG/UR/HMGU), C. Radischat (UR), J. Schnelle-Kreis (HMGU), C. Schön (TFZ), H. Hartmann (TFZ), R. Zimmermann (UR/HMGU)

An investigation was performed for the comprehensive characterisation of organic compounds emitted from wood combustion and the impact of combustion conditions on their formation. For the first time, both gaseous and particulate organic compounds were determined simultaneously with REMPI-TOF-MS and AMS. This approach allowed the observation of the fast and highly dynamic changes in the formation of multiple aromatic hydrocarbons, such as phenols and PAH during different combustion phases.

Various hazardous compounds, such as phenols or polycyclic aromatic hydrocarbons (PAH) and particulate matter (PM), originate from incomplete combustion processes of organic matter. Studying combustion aerosol by offline filter or impactor sampling of particles followed by lab analysis is a common procedure in aerosol research. In this study, an approach was performed towards a more comprehensive characterisation of combustion aerosols. The combination of different techniques not only allowed the characterisation of collected particles, but also a combined characterisation of particulate matter and gas-phase. The reaction mechanisms of combustion in real-time was intended. For this approach, online-measurements (Fig. 1) were carried out by resonance enhanced multi photon ionisation (REMPI) time-of-flight mass spectrometry for analysing volatile aromatic compounds (VOCs). The PM, fraction was analysed simultaneously by high resolution time-of-flight aerosol mass spectrometry. The online measurements were supported by offline sampling of particulate matter on quartz fibre filters for later analysis of organic and inorganic compounds. Two sampling points were located after the dilution tunnel to allow condensation of semi volatile organic matter on particles by dilution and cooling of aerosols to temperatures below 50 °C. The whole combustion process from ignition to burn-off was covered. The end of a sampling duration was indicated by the wood mass loss of at least 96 %. Emissions from a logwood boiler and a stove were investigated. Different types of wood, i.e. spruce and beech with different moisture contents, were investigated. In this report experiments including operation errors, such as fuel overload or air deficiency compared to normal combustion condition of beech wood in a log wood stove, are presented.

Experimental

REMPI-TOFMS
The sampling point of the REMPI-TOFMS was located close to the stove in the undiluted raw exhaust pipe. This enables direct probing of volatile gases with almost no aging reactions or other compound modifications. The used technique, i.e., resonance enhanced multi photon ionisation (REMPI), is selective and sensitive for phenols and mono and polyaromatic hydrocarbons (PAHs). Mass to charge ratios in a range from m/z 20
to m/z 320 were recorded on-line and in real-time with a time resolution of 0.5 s.

**HR-TOF-AMS**

Online analysis of the aerosol composition of non-refractory compounds in the PM$_1$-particle size range was carried out by a high resolution time-of-flight aerosol mass spectrometer (HR-TOF-AMS) with a time resolution of 10 s. The aerosol mass spectrometer sampled after the dilution tunnel and, depending on particle concentrations, up to three additional ejector diluters with 1/10 dilution each were interconnected.

**Offline sampling**

Filter samples were taken for analysis of inorganic and organic constituents. Analysis was carried out with in-situ derivatisation thermal desorption gas chromatography time-of-flight mass spectrometry (IDTD-GC-TOFMS) [2].

**Results and Discussion**

In the following section three different experiments of beech wood combustion and their dynamic are compared. These experiments were carried out under different combustion conditions: normal (Exp. A), overloaded (Exp. B) with i.e., a triple of the manufacturer’s recommended fuel amount, and oxygen-deficient (Exp. B) with less air supply. Based on the chemical composition of the emissions a complete burn-off was separated in four parts...
specific combustion phases. The first two phases were classified according to changes from compounds measured by the REMPI-TOFMS in a pyrolysis phase (P1) and in a harsh combustion phase (P2). The third phase, a stable flaming phase (P3), ends with the burn-off phase (P4) indicated by a strong increase of the carbon monoxide concentration.

i) REMPI-TOFMS

The concentration profiles from three experiments with different combustion conditions are shown in figure 2. Under normal conditions [Exp. A, Fig. 2 (A)] starting phase P1 holds up 1.5 min and was dominated by phenolic compounds, such as phenol and guaiacol, and maximum yields of PAH. The following combustion phase P2 featured a slow decrease of phenolic and aromatic compounds, which indicates a moderate combustion. In the third phase P3, which began after 14 min, only small concentrations of phenol could be detected. During the last phase P4 even phenol was no longer detectable. An overload of fuel (Exp. B) resulted in maximum compound yields [Fig. 2 (B)]. Again, P1 was dominated by pyrolysis products, such as guaiacol (m/z 124). A severe combustion phase P2 followed after 10 min. It ranged over 25 min and was characterised by maximum yields of aromatics, such as naphthalene (m/z 128) and phenol (m/z 94). The progress of P3 and P4 was comparable to the progress of Exp. A. It must be considered that the air supply partially varied during the experiments to support the ignition of the fuel. In regard to this observation, the realisation of the third experiment (Exp. C) proved to be difficult. Without air supply no ignition took place and the fire went out. The change of the air supply is denoted in figure 3 C. 0 % air supply means that air reaches the combustion zone only through the leaks of the stove housing, whereas an air supply of 50 % is recommended for the continuous operation by the manufacturer. However, it can be observed that air deficiency resulted in a longer phase P1, i.e. 10 min. The following phase P2 exhibited a moderate combustion with slightly higher PAH yields as compared to the yields from Exp. A. The trends of P3 and P4 were similar to the trends of Exp. A and B. A remarkable change from pyrolysis to combustion conditions was observed in Exp. C (start of P2), which was indicated by a decrease of guaiacol and an increase of naphthalene.

ii) HR-TOF-AMS

AMS results of the experiment under normal conditions (Exp. A) are shown in figures 3 and 4. Figure 3 illustrates the time series of concentrations from the non-refractory compounds in the four different combustion phases. The averaged mass spectra of these phases are provided in figure 4. The organic fraction with approximately 95 % generally has the biggest impact on the aerosol composition. This impact decreased during the different phases (Fig. 3), so the contribution of the organic mass yielded 99 % in the pyrolysis phase (P1) and approx. 83 % in the burn-off phase (P4). In this latter phase the contribution of nitrate fraction increased, whereas other inorganic anions, chloride and sulphate, mainly contributions during the regular combustion phases (P2 and P3). The mass to charge ratio (m/z) 60 which derives, as an important fragment, from anhydrous sugars, especially from the wood combustion marker levoglucosan, is important for ambient studies [1]. The signal of m/z 60 decreased during the phases P1 and P2 and was almost stable with a low abundance during phases P3 and P4; this suggests that in later phases of combustion most of the levoglucosan precursor cellulose was converted. The phenolic compound relevant masses increased, especially in phases P2 and P3, as observed in the REMPI measurements. The experiments
Figure 2 | Concentration of four selected compounds. Phenol, guaiacol, naphthalene and phenanthrene obtained under three different experimental conditions in a stove.

under non-optimal use (Exp. B and C) obtained similar compositions, but they provided an important change in the emitted mass concentration. For example, the emitted organic mass concentration is standardised to the experiment time and amount of fuel. It is around 3.8 times higher for the overloaded experiment (Exp. B) and 4.2 times higher for the oxygen-deficient experiment (Exp. C). The mass spectra at the different combustion phases showed higher variations during the phases. For example, the higher masses (higher than 100) increased much more strongly. Especially in phase P2 under the overloaded conditions, the higher and lower masses had a similar concentration. Compared to the experiment under normal conditions (Exp. A), the signal of m/z 60 in the oxygen-deficient experiment (Exp. C) had a higher but constant concentration during all combustion phases. This indicates that more evaporation of the levoglucosan takes place instead of combustion.
Figure 3 | AMS time series from the normal beech log wood experiment (Exp. A) of two non-refractory submicron aerosol components including organic mass (green), nitrate (blue), sulphate (red), and ammonium (orange) with a 10 second time resolution.

Figure 4 | AMS compound coloured mass spectra from the normal beech log wood experiment (Exp. A) of the four different combustion phases: the P1 pyrolysis phase, the P2 harsh combustion phase, the P3 stable flaming phase, and the P4 burn-off phase.
### iii) Offline sampling

Contrary to the online measurements, the following results refer to a complete burn-off. This also allowed the determination of PM mass emitted by burn-offs of the different experiments. At regular combustion conditions (Exp. A) 100 mg m⁻³ PM were emitted (Fig. 3). The exhaust temperature in Exp. A was 300 °C on average. Figure 3 also shows that overall sums of different compound groups were significantly lower compared to results of maloperation. Although concentrations of most organic compounds were two or three times lower than in Exp. B and C, critical amounts of higher PAH, like Benz[a]pyrene (BaP) (10 µg m⁻³), could still be found. As observed in the online measurements, the composition of PM differed substantially when comparing the different combustion experiments. The emitted organic matter from the overload experiment (Exp. B) was dominated by PAH and oxygenated PAH (o-PAH). The mass fraction of these measured hazardous compounds was 12 % of total PM. A more than critical concentration of BaP was found (430 µg m⁻³). The conditions in Exp. B with high combustion temperatures (exhaust temperature was 530 °C) favoured the formation of higher PAH. Due to the overloaded combustion chamber and high demands of air, the reaction time is too short for post-combustion of PAHs. When considering the results of the REMPI-TOFMS measurements in the hot raw exhaust, it must be assumed that the formation of PAH took place even after the exit of the combustion chamber within the hot raw gas. As a result, high amounts of hazardous PAH and o-PAH were released to the atmosphere. The total PM mass rose up to 220 mg m⁻³.

The PM emissions from combustion with deficiency of oxygen (Exp. C) had similar values (200 mg m⁻³), like the combustion with overload. Thus the total PM mass was about two-fold higher when compared to regular combustion conditions. Contrary to Exp. B, emissions of combustion with air deficiency were predominated by degradation products of lignin (16 % of PM) and cellulose/hemicellulose (11 % of PM). As observed in the AMS measurements, the anhydrous sugars levoglucosan, galactosan (Fig. 5) and mannosan were not combusted completely. The concentrations of all PAHs were lower compared to Exp. B. The averaged concentration of Benz[a]pyrene was 110 µg m⁻³. Interestingly, compounds like 3,3',5-Trimethoxy-4,4'-dihydroxystilbene were only observed in experiments with air deficiency. It seems that these phenol-dimeres are not further decomposed to phenols, which is due to the lack of oxygen. Generally, the absence of oxygen is responsible for the formation of large amounts of such

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**Figure 5** | A selection of compounds and compound groups. On the top chart illustrated as percentage of total PM. **Below**: total concentrations of PM and selected compounds.
intermediates at low temperatures. The
exhaust temperature in this experiment
was only 270 °C. Phenols derived from the
lignin structure in particular are discussed
as possible precursors for PAH [3]. In the
case of of air deficiency, these reaction
sequences seem to be interrupted.

**Conclusions**

The data analysis and their combination
allowed the separation of four different
combustion phases according to

**Funding and Cooperation:** The project was accomplished and supported by the Technology and
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Laser-Desorption as a Technique for the Detection of Security-Relevant Substances Via Online Soft Ionisation Ion Trap MS

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Ambient laser-desorption coupled to a soft ionisation source equipped multi dimensional ion trap mass spectrometer is a powerful device for the analysis of organic substances on surfaces, especially those with a very low vapour pressure. Laboratory and field test scenarios were performed in cooperation with the German Federal Criminal Police Office, where the applicability was demonstrated for various explosives, drugs and drug precursors, such as TNT, Tetryl, HNS, cocaine, amphetamine, phenylpropanone and safrole. Fast online measurement and high selectivity can be guaranteed by the soft ionisation technique associated with the MSn possibility of the ion trap mass spectrometer.

Considering current security issues, there is a requirement to have a powerful tool for the detection of security relevant substances, e.g., traces of explosives and drugs/drug precursors related to clandestine laboratories. One of the biggest challenges in detecting or investigating security relevant substances, especially explosives, is frequently the very low vapour pressure and the instability of the target molecules. Ambient desorption and ionization techniques facilitate a fast and easy sampling of surface adsorbed analytes [1]. To increase the flexibility of the desorption and to expand the possibilities for ionization these processes can be separated. Laser desorption under ambient pressure in an inert gas coupled with a GC separation can be found in a number of experiments and applications [2]. Hence direct laser-desorption at ambient conditions is an eminent alternative to transferring a surface adsorbed substance into the gas phase for detection. In contrast to a thermal desorption, where the sample must be evaporated and may be destroyed by the thermal input, the laser desorption disperses the sample explosively from the surface [3]. Due to the short duration of the single laser pulse in a nano-second scale, a thermal intake to the target molecule can be minimized. Technical aspects and optimization steps, such as type of laser, wavelength, energy density or coupling between desorption and analysis parts were investigated in laboratory scale. Primary target compounds were explosives, drugs and their precursors. Whereas the wavelength exhibits only a minor effect on the desorption process, pulse duration and energy input are essential parameters. In the case of the laser desorption unit, the development leads to a fiber coupled pulsed Nd:YAG-laser working at 532 nm, with a pulse width of 4 ns and energy densities up to 100 MW/cm² depending on the substance as well as surface material and its structure. For the idea of a fast online measurement system, a fast detector is essential. To avoid a sample preparation or a time-consuming preseparation in a GC, an ion trap mass spectrometer is used that was developed in a previous project [4]. The advantage of this procedure is the MSn functionality in connection with a soft ionization
technique to guarantee a high selectivity. Aligned to a practical use in real scenarios, the concept of laser-desorption could already demonstrate its strengths in measurements of forensic relevant substances. Laboratory and field test scenarios were performed in cooperation with the German Federal Criminal Police Office where the applicability could be demonstrated for various explosives, drugs and drug precursors such as TNT, Tetryl, HNS, cocaine, amphetamine, phenylpropanone and safrole. A wide range of samples and matrices have been investigated successfully, ranging from artificial ones, e.g. on aluminium foil or polystyrene carrier to real crime scenario samples, like used cases, leather or metal surfaces. As part of the development process, different designs of the laser desorption unit were tested and evaluated. Thus a sensitivity enhancement could be reached as a result of the increased encapsulating level of the laser desorption head. Starting with the third version, the laser fiber coupling was implemented. In laboratory-based experiments of the selected explosives and precursors, limits of detection (LOD) in a low nanogram range could be determined via laser desorption under ambient condition coupled with NCI-ITMS detection. A context for their vapour pressures is still evident. The substances Nitrobenzene and EGDN could be measured directly from the gas phase by their vapour pressure

Figure 1 | Modular multi sampling LD-SPPI/CI-IT-MS system. During measurement of MDMA (Ecstasy) high pressure synthesis reactor via endoscopic probe.

Figure 2 | Right: Sample preparation with double packed TNT in exposure time of 1h in the closed briefcase; measurement of TNT traces on the leather surface of the exposed briefcase; camera equipped endoscopic laser desorption probe head with the detection of TNT traces; top: MS/MS spectrum of TNT traces in briefcase; left: Sampling on an engineer’s pliers; spectrum of laser desorption PCI-ITMS measurements of a pliers normally used in the toolbox of an explosion test ground with supposed traces of TNT on mass 227 [m/z] and Tetryl with the first fragment at 243 [m/z].
at room temperature. In the case of 2,4 Dinitrotoluol a LOD of 3 ng, for TNT 4.5 ng and for Tetryl a LOD of 30 ng could be observed. Parallel to the increasing LOD the corresponding vapour pressure decreases from approx. 3 e-3 mbar for 2,4-DNT, 2.4 e-4 mbar for TNT down to 3.8 e-10 mbar for Tetryl. According to the common definition of the LOD a signal to noise ratio of at least 1:3 is assumed for a successful detection. All ascertained LOD values are based on real measurements and the mentioned minimum in S/N ratio. For the final test a modular designed demonstration system as pictured in figure 1 had been set up. Multiple sampling opportunities are integrated for volatile and less volatile substances (endoscopic direct probe for volatiles and for less volatiles the endoscopic laser desorption unit or thermal desorption with SPME fibers or wipe pads). The detector unit (Ion Trap MSn) can be switched between SPI, CI as soft ionization techniques and even EI ionization. The TNT detection on leather parts of a briefcase as displayed in figure 2 was performed with the LD probe in NCI MS/MS mode of the Ion Trap. The briefcase had been prepared with TNT in a double packed plastic bag that laid in there for one hour under constant ambient conditions. The sampling area had no direct contact with the TNT package. The signal could be attached via MS/MS doubtless to TNT with the molecular ion signal at 227 [m/z] and fragments at 210 and 194 [m/z]. The observed signal/peak dissemination is a direct effect of the ambient air intake by the sampling probe and a resulting variation in CI ionization. A further measurement is also shown in figure 2. The investigated object is an engineer’s pliers normally used in a toolbox on an explosion test ground. On the basis of the mass signals in the positive CI-IT-MS spectrum at 228 [m/z] and 243 [m/z] traces of TNT and Tetryl could be assumed. Beside the shown examples various drugs and drug precursors could be detected within this measurement campaign. Figure 3 shows measurements of amphetamine and cocaine on laboratory gloves and court exhibits. Laser desorption at ambient

Figure 3 | Left: LD supported measurement of amphetamine on laboratory gloves after opening a test tube and cleaning the gloves with tissues detected via PCI-ITMS; right: LD measurement of cocaine on a contaminated leather jacket used for smuggling detected via PCI-ITMS.
conditions coupled to a soft ionization source equipped MSn mass spectrometer is a powerful device for the analysis of substances on surfaces, especially those with a very low vapor pressure. A fast online measurement is enabled without a significant loss of selectivity because a time consuming sample preparation and separation such as GC is not required. The high selectivity can be guaranteed by the soft ionization technique associated with the MSn capabilities of an ion trap mass spectrometer.

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A better understanding of the chemical composition of organic carbonaceous material from tropospheric aerosol is very important with respect to climatic and health research. In this regard, the study of the organic fraction of aerosol particles and their specific health effects are gaining increasing interest, but the identification of the carbonaceous fractions on a molecular level still provides an analytical challenge. The application of thermal/optical methods for the determination of the overall content of organic and elemental carbon (OC and EC fractions) by desorption, pyrolysis, and oxidation enables the detection of chemically different bonded carbon as non-specific sum parameters.

This is done by releasing the carbonaceous portion of particulate matter (PM) sampled on filter with a succession of temperature steps from approx. 100 °C to 850 °C (e.g., 120 °C, 240 °C, 450 °C, and 550 °C for organic carbon fractions, referred to as OC1, OC2, OC3, and OC4, respectively). The evolved gases are oxidized to CO2, which is catalytically reduced to methane in a second step and subsequently measured by a flame ionization detector. A He/Ne laser is employed to determine the reflectivity and transmission to account for the part of OC that is transformed to char initially. By doing this, the distinction between OC and EC fractions is improved. A novel analytical technique was developed, by which this thermal analytical method was hyphenated with a photo ionization mass spectrometer. Thus, a direct chemical analysis of the evolved products is possible. Figure 1 shows a scheme of the setup of the coupling. Prior to the oxidation unit, a small amount of the desorbed gaseous species is side-lined to the ion source of the mass spectrometer via a heated deactivated quartz capillary.

Thus the EC/OC measurement can proceed undisturbed. Due to the nature of the applied soft photo ionization, the molecular ion pattern of each carbonaceous fraction can be obtained. The assembly is described in detail elsewhere [1]. Figure 2 shows a two-dimensional depiction of the whole EC/OC analysis of an urban aerosol sample representing roughly 1 m3 of air, where single photon ionization time-of-flight mass spectrometry (SPI-TOFMS) has been employed. This ionization method is used for detection of a wide range of substances and has a high sensitivity, thus reflecting the aromatic and aliphatic pattern of each carbonaceous fraction and its changes along the course of the
The observation [made with REM-PI (see previous annual report)] that most of the detectable organic species are released in OC2 and OC3 is also true for SPI. This means that the bulk of all-phatic compounds emerge at these temperatures, too. In contrast to the REMPI measurements the molecular pattern is shifted to smaller molecules. These are mainly aldehydes, furan derivatives and esters or acids as can be seen in Figure 3. Characteristic masses of the OC3-step of the cellulose and lignin decomposition can be assigned to the spectrum of the ambient sample. The peaks that are marked with red bars in Figure 3 are connected to the decomposition of cellulose. These are, for example, m/z 42 (propene), 44 (acetaldehyde), 58 (acetone), 68 (furane and iso-prene), 84 (cyclopentanone), 96 (dimethylfurane and furfural) and 110 (catechol and hydrochinone and methylfurural). The green bars show the decomposition products of lignin (see Figure 3), which are, for example, m/z 94 (phenol), 108 (methylphenol), 124 (guaiacol), 138 (methyl-guaiacol), 150 (vinyloguaicol) and 152 (ethyl- or formylguaicol). Thus analysis of ambient filter samples, in combination with the investigation of cellulose

Figure 1 | Scheme of the thermal/optical carbon analyzer. Includes its coupling to photo ionization mass spectrometry.

Figure 2 | Two-dimensional SPI/TOF-MS-spectrum of an ambient filter.
and lignin, revealed a large influence of wood combustion on the ambient sample. Therefore, the particles of wood combustion were investigated as well. The mass spectrum of the OC3 fraction is shown in Figure 4. As mentioned above, a lot of lignin breakdown products can be found in the wood sample. Guaiacol (m/z 124), methylguaiacol (m/z 138), vinylguaiacol (m/z 150) and formylguaiacol (m/z 152) can be seen in all OC steps. Furthermore, some aromatics, primarily phenanthrene and pyrene, can be observed in the OC1 and OC2-step. Guaiacol and its derivates were also the dominant signals in the REMPI-spectra of the OC steps. With REMPI also retene, a wood marker, was detected. In the OC4-step (spectrum not shown) some cellulose products, such as methylfurane...
(m/z 82), dimethylfurane or furfural (m/z 96) and catechol, hydrochinone or methylfurfural (m/z 110) can also be found. These facts confirm the strong impact of wood combustion on the organic constitution of the ambient sample. In the future measurements will be carried out with both ionization techniques to investigate the composition of oligomeric structures on airborne particulate matter.

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Concentrations and Source Contributions of Particulate Organic Matter Before and After Implementation of a Low Emission Zone

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Samples of PM2.5 were collected at the monitoring site in Lothstrasse before and after the implementation of the LEZ from October 2006 to February 2007 and from October 2009 to February 2010. The Lothstrasse is located within the LEZ, allowing for a thorough monitoring of the LEZ implementation effect upon the reduction of hazardous, particle-associated organic substances and the different sources of PM pollution.

The most severe environmental problems in Munich are caused by traffic. Many heavy duty vehicles make their way through the city of Munich because there is no complete highway ring round Munich. For traffic and transport management this is the main problem of the future. In spite of the fact that about 781,000 cars are licensed in Munich, the modal split is comparatively good. The traffic volume during peak hours and also off-peak hours is very large. Low emission zones (LEZ) are areas in which vehicular access is restricted to vehicles that emit low levels of air pollutants only. In 2008, a LEZ was established in the inner city of Munich, Germany, in order to pursue the reduction of pollution. Organic compounds of biogenic and anthropogenic origin often represent a large fraction, up to 40%, of total PM mass. To protect both human health and the environment, it is important to combat pollutant emissions at the source and to identify and implement the most effective reduction measures at local, national and international levels. Comprehensive studies are therefore necessary to evaluate the characteristics of PM at the different sources[1]. The sampler of PM$_{2.5}$ was located within the LEZ at the monitoring site at Lothstrasse (latitude 48° 9' 16'' N; longitude 11° 33' 17'' E). Samples were collected every third day from October 2006 to February 2007 and from October 2009 to February 2010. A total of 80 samples were collected during these two periods before and after the implementation of the LEZ. The participation at the sampling site “Lothstraße” allows the characterization of representative, health relevant organic substances by investigating concentration courses, evaluating influencing parameters like meteorology, sources, source variabilities and long range transport in a representative urban area. The samples were analyzed for particulate

Figure 1 | Location of the sampling site in Munich.
organic compounds (POCs) by in-situ derivatization thermal desorption gas chromatography time of flight mass spectrometry (IDTD-GC-ToF-MS)\(^2\). More than 80 organic species were analyzed, including PAH, oxidized PAH, n-alkanes, iso & anteiso alkanes, hopanes, resin acids, fatty acids, anhydrous sugars and phenolic compounds. Nitro PAHs were analyzed by high-performance liquid chromatography-fluorescence detection. Elemental and organic carbon fraction (EC and OC) were analyzed by thermal-optical analysis (IMPROVE-A protocol)\(^3\) at Desert Research Institute (DRI), Nevada, USA.

The box plots depicted in figure 2 visualize that there are no significant differences for the sum of PAH, sum n-alkanes and 1-nitropyrene concentrations between 2006/7 and 2009/10. As opposed to this, differences for the sum of hopanes, the sum of O-PAH and levoglucosan are observable with higher concentration levels in 2009/10, showing an unexpected behavior with respect to the LEZ effect. On the other hand, lower concentrations for 2-nitropyrene, 2-nitroflouranthene and EC were found in 2009/10.

To obtain more detailed insight into the contribution of different sources of particulate organic compounds (POC), positive matrix factorization (PMF)\(^4\) was applied as a multi-variate source apportionment model. More than 60 organic species were used in PMF analysis, including PAH, oxidized PAH, n-alkanes, iso & anteiso alkanes, hopanes, resin acids, fatty acids, anhydrous sugars and phenolic compounds. The PMF analysis with four factors afforded the most reasonable interpretation of the source profiles, which were related to primary PM emission sources. The factors are dominated by the pattern of a single source or groups of sources with similar variation in time of the emissions. In the first factor, the influence of the vehicular emission source is predominant. 55-85% of hopanes with mineral-oil-based pattern (homohopane index of 0.49) and n-alkanes (CPI of 0.78) are associated with this factor. The second factor is characterized by a compound pattern which represents a mixture of tobacco smoke (iso & anteiso alkanes and n-alkanes with CPI of 2.13), cooking emissions (fatty acids) and traffic (homohopane index of 0.59). In the third factor, about 10-85% of PAH and 15-45% of oxidized PAH are associated beside the hopane pattern (homohopane index of 0.22) which is similar to emissions from brown coal combustion. The last factor is characterized by a pattern which represents a wood combustion source. 60% of levoglucosan, 59% of dehydroabietic acid, 60% of retene and 40-80% of the oxidized PAH are associated with this factor. Differences in contributions were seen between the two sampling periods for all factors. For

Figure 2 | Box plots for some organic compounds and EC before and after the LEZ.
example, a high contribution of the first factor is noticed in the second sampling period. This is most probably due to some construction activities near the sampling site. The impact of wind direction (WD) and wind speed (WS) was also considered. WD and WS were very similar in both sampling periods. No significant effect of wind direction and speed, neither on POC concentrations nor on the contribution of the source factors, was observed. The results from the two sampling periods, besides the source apportionment study using a PMF model, indicates that the implementation of LEZ had no clear reduction effect on neither the concentrations of POC nor on the pollution sources. This may be due to some unusual events or activities, especially during the second sampling period in 2009/10. A further investigation on those unusual activities and corresponding days is currently undertaken. Data from a third sampling campaign in 2011/12 will be included in further analyses.

**Funding and Cooperation:** The EC/OC analysis was performed in cooperation with the Desert Research Institute (DRI) in Nevada, USA.


Identification of Fentanyl Derivatives at Trace Levels with Non-Aqueous Capillary Electro-phoresis-Electrospray-Tandem Mass Spectrometry (MS^n, n = 2, 3): Analytical Method and Forensic Applications

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The coupling of non-aqueous capillary electrophoresis (NACE) with electrospray ionisation mass spectrometry (ESI-MS) as a powerful tool for the identification and trace analysis of fentanyl derivatives was demonstrated. Forensic applications and model experiments were performed successfully.

Fentanyl is a synthetic opioid which is used in anesthesia to control pain. Its narcotic analgesic potency is about 80 times that of morphine and 50 times that of heroin. Several derivatives with different efficiencies like sufentanil or methylfentanyl were developed. Beside their therapeutical application there is an abuse of these compounds as illicit drugs in the drug scene. The use of carfentanil (potency > 100 times higher than that of fentanyl) as a psychotoxic combat agent has been suspected. In 2002, when Russian military disburdened 830 hostages in a musical theatre in Moscow, they presumably used a fine aerosol

Figure 1 | CE-MS run of six fentanyl derivatives. separation voltage: 28 kV. a: Buffer: aqueous solution of formic acid 100 mmol/l and isopropanol 10% (v/v); b: Buffer: aqueous solution of formic acid 200 mmol/l, ammonia 7 nmol/l and acetonitrile 10% (v/v); c: Buffer: non-aqueous solution of ammonium acetate 200 mmol/l 30% (v/v) and acetonitrile 70% (v/v); d and e: Buffer: non-aqueous solution of ammonium acetate 200 mmol/l 10% (v/v) and acetonitrile 90% (v/v); injection 4 s, 3.45 kPa, capillary: 50 µm I.D (d: 75 µm I.D.), length 80 cm, sheath liquid isopropanol/water (1:1 v/v), positive ion mode.
of carfentanil to overbear the hostage-taker. 127 humans died. The standard techniques for the analysis of fentanyl are GC/MS, spectroscopic techniques and LC/MS. Capillary electrophoresis (CE) has proven to be a highly suitable technique for the analysis of drugs of abuse due to its high separation efficiency, high matrix tolerance and short analysis time. The combination of CE with MS presents a powerful tool for the investigation of complex samples. In figure 1 results of the development of the separation system for the analysis of six fentanyl derivatives via CE-MS is visible. Limits of detection of about 1 nmol/l were found for ESI-MS detection in the positive ion mode. Thus the sensitivity of the procedure is adequate for the reliable detection of fentanyl derivatives at trace levels. The linear range over more than three magnitudes with a correlation of $R^2 > 0.99$ is shown. Repeatability measurements yielded RSD between 0.00 % and 0.07 % with normalisation to the two internal standards fentanyl-D5 and car-fentanil-D5 for the migration time.

An extract of a synthesis residue seized in a clandestine fentanyl laboratory in Darmstadt, where a former winner of the "Jugend forscht" competition synthesised fentanyl in a kitchen-lab, was analysed with the developed procedure. In the mistaken belief that it was heroin, a 32 year old female drug consumer died because of a wrong dosage and the high potency of fentanyl. For our analysis, 21 mg of a light-blue liquid that was seized in a synthesis-flask in the kitchen-lab were dissolved in 500 µl methanol spiked with fentanyl-D5 (35 nmol/l). The resulting solution was diluted 1:3 with water and directly injected into the separation capillary. In the upper line in figure 2 the base peak electropherogram (BPE) for this non-aqueous capillary electrophoresis (NACE) ESI-MS run is shown, but no characteristic peak is visible. Traces of fentanyl are only detectable in the respective reconstructed electropherograms for 337.3 m/z (fentanyl) and 342.4 m/z (fentanyl-D5). In this real sample, fentanyl was doubtlessly identified as a trace component via the migration time, the deuterated standard, the mass spectrum and the MS-MS-

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**Figure 2 | Left:** NACE-MS run of an extract of a synthesis residue seized in a clandestine fentanyl laboratory in the SIM mode (base peak electropherogram: 335 – 425 m/z) and the reconstructed electropherograms of fentanyl (337.3 m/z) and fentanyl-D5 (342.4 m/z); **Right:** the corresponding MS1- (upper spectrum) and MS2-spectrum (lower spectrum) at 5.8 min, positive ion mode (for experimental parameters refer to Figure 1e).
experiment. Hence the high potency of the developed NACE-ESI-MS procedure for the trace detection of fentanyl has been demonstrated. Furthermore, we conducted a model experiment to test the suitability of the developed procedure for the trace detection of carfentanil on contaminated textile surfaces, because the analysis of clothing is one important part of the forensic science investigation. Therefore, 10 ml of a 2.5 µmol/l solution of carfentanil were nebulised on a garment tatter (size: 6 x 4 cm). The dried garment sample was extracted in 25 ml of a 0.6 µmol/l methanolic carfentanil-D5-solution by ultrasonication for 15 minutes at 40 °C. The solution was then diluted 1:10 with water and directly injected into the capillary. The reconstructed electropherogram for this sample and the corresponding MS and MS-MS-spectra are shown in figure 3. It is obvious that the developed procedure is well-suited for the identification of carfentanil contaminations on a textile matrix.

Figure 3 | left: NACE-MS run of a homemade carfentanil sample in the SIM mode; right: corresponding MS1-spectrum (upper spectrum) and MS2-spectrum (lower spectrum), positive ion mode (for experimental parameters refer to figure 1e).

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Phosphorylation of proteins is an important regulation mechanism in living cells. Hence analysis of phosphorylated sites in proteins is important for the understanding of biological systems. To evaluate the power of the analytical procedures and instruments we focus here on the analysis of stathmin, a well characterized 17kDa protein that is important for the regulation of microtubule formation. Samples were extracted from rat brain tissue and isolated by two-dimensional gel electrophoresis and tryptic in gel digestion. Phosphopeptides were enriched by metal oxide affinity chromatography (MOAC) on TiO₂ surfaces. In brief, protein digests were applied with binding buffer and after washing off all non-bound compounds, the phosphorylated peptides were eluted using a 0.25 % NH₄OH-solution. Samples were prepared for MALDI analysis according to [1]. Figure 1 shows the adsorption mechanism and the proposed side reaction, leading to partial dephosphorylation during the desorption step. Mass spectrometric analysis (see Eickner et al., 2011) was carried out by MALDI-TOF-MS and MALDI FT-ICR-MS on our newly installed 7T Solarix instrument (Bruker). The FT-ICR mode was set to broadband, 1MSamples, 1.95 s FT-transit (ICR-Time) with a laser power of 32 % at 200 Hz and ultra-large spot size. The resulting resolution was about 80,000 at m/z 1621. Mass spectrum and partial sequences of tryptic digested stathmin peptides are shown in figure 2. The high mass resolution and accurate mass assignment (error ≈ 0.2 ppm after internal calibration) allowed the exclusion of the presence of N-terminal acetylated peptides in the sample [1]. The high-
Figure 2 | High-mass resolution MALDI FT-ICR mass spectrum of peptide mixture of the stathmin-derived tryptic peptides upon phosphopeptide enrichment on TiO$_2$ tips with citric acid (20 mg mL$^{-1}$) and DHB/THAP mix as matrix. The ion signals are assigned to partial sequences [shown in parentheses] from mature rat stathmin. +P indicates phosphorylation.

Figure 3 | MS/MS spectra of isolated $m/z=1621$. The dominant ion signal results from loss of phosphoric acid. Y$^-$-ions and B-ions are labeled and their locations in the partial sequence are depicted.
resolution spectrum clearly showed that the mixture contained phosphopeptides with some non-phosphorylated sibling peptides. The presence of non-phosphorylated peptides in the mass spectra upon phosphopeptide enrichment confirms the proposed dephosphorylation reaction during basic desorption (Fig. 1). Moreover, as the ratio of phosphopeptide to non-phosphorylated sibling varied phosphopeptide dependent, these analysis results may be used to estimate stability differences of phosphorylation sites in individual proteins, possibly adding valuable information on biological regulation processes. The position of the phosphorylated serine site of the [27-40]-phosphopeptide was investigated using the MS/MS capability of our instrument. In figure 3 the obtained MS/MS of parent ion m/z=1624 is shown. The isolation window was set to 10 u, and the collision energy to 45 V. Collision-induced dissociation (CID) was performed using argon as collision gas in the collision cell that is located between the quadrupole and the FT-ICR cell. The MS-fragment Y9" clearly indicates the third serin of the [27-40]P-peptide as phosphorylation site - in compliance to literature data.

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Prof. Dr. K.-H. Meiwes-Broer, PD Dr. J. Tiggesbäumker, Dr. V. von Oeynhausen, Dr. I. Barke, Dr. S. Fiedler, Prof. Dr. S. Lochbrunner, Prof. Dr. R. Redmer
www.physik.uni-rostock.de/cluster

Proteome Center Rostock
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www.sciencenet-mv.de/index.php/kb_1785/pb_117/pb.html

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Institute of Chemistry
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Prof. Dr. A. Cappiello
Public and State Institutions

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Belluno, Italy
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Bavarian Research Foundation (Bayerische Forschungsstiftung)
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www.forschungsstiftung.de/

Bayerische Landesanstalt für Wald und Forstwirtschaft (LWF)
Freising, Germany
Dr. H.-P. Dietrich
www.lwf.bayern.de/

Bundeskriminalamt (BKA)
Wiesbaden, Germany
Dr. M. Pütz, Dr. R. Schulte-Ladbeck
www.bka.de

Federal Environment Agency Austria (Umweltbundesamt)
Vienna, Austria
Dr. Weiß
www.umweltbundesamt.at

Federal Environment Agency Germany (Umweltbundesamt)
Global Atmosphere Watch (GAW) - Globale Überwachung der Atmosphäre
Garmisch-Partenkirchen, Germany
Dr. L. Ries
www.umweltbundesamt.de
JMSC Co-Workers
**Dr. Gülcin Abbaszade, Dipl.-Chem.**  
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Development and validation of analytical methods for chemical particle characterisation; quantification of health-relevant substances in ambient aerosol particles.  

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Development and validation of an analytical system for thermal analysis (TA) coupled with evolved gas analysis (EGA) via mass spectrometry (MS) using photo ionisation (REMPI and SPI) and electron impact ionisation (EI).  

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**Dr. Matthias Bente, Dipl.-Phys.**  
Photonion GmbH  

**Scientist**  
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Christian Busch, Dipl.-Chem.
University of Rostock / Helmholtz Zentrum München

PhD Student

Fundamental investigation of the transient pyrolysis and combustion processes in cigarettes by application of a cigarette combustion simulator. On-line, real-time analysis of organic combustion by-products is performed by photoionisation mass spectrometry (SPI/REMPI-TOFMS).

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Michael Clausen
Helmholtz Zentrum München

Technician

Sample preparation and GC-MS analysis of target components in aerosols. Analysis of health-relevant organic substances in environmental substances.

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George-Constantin Dragan, Dipl.-Ing.
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Development, setup and construction of a work place aerosol simulation unit, consisting of an aerosol generator, a flow tube reactor and an aerosol chamber.

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Sven Ehlert, Dipl.-Chem.
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PhD Student

Detection of security relevant substances (explosives, narcotics, toxics and the related precursors) using Laser Desorption Mass Spectrometry. Short Laser Pulses are used for atmospheric pressure ablation of analytes from surface.

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**Michael Elsasser, Dipl.-Chem.**  
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Stationary and mobile aerosol measurements with a high time resolved online aerosol mass spectrometer (AMS) in ambient and smoke chamber assays for determination of wood combustion markers in ambient aerosol.

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**Sabrina Erdmann, Dipl.-Biol.**  
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Application of gas chromatography and mass spectrometry for the analysis of complex samples.

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**Markus Eschner, Dipl.-Chem.**  
Helmholtz Zentrum München / ASG  
*Guest Scientist*

Development and investigation of multi-dimensional separation techniques based on the coupling of single-photon ionisation (SPI) mass spectrometry (MS) to gas chromatographic methods (GC, GC×GC) for on-line and off-line applications.

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**Ernst Feicht, Dipl.-Ing. Agr.**  
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Characterisation of ambient aerosols. Running of aerosol characterisation and sampling sites in Munich and Augsburg.

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Alois Fendt, Dipl.-Chem.
University of Rostock

PhD Student

Investigation of biomass pyrolysis gases via time-of-flight mass spectrometry (TOF-MS) using two soft photo ionisation techniques (SPI and REMPI) as online detection method for organic compounds at a technical flash pyrolysis plant.

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Dr. George A. Ferron, Dipl.-Phys.
Helmholtz Zentrum München

Associated Consultant

Modelling of the deposition of hygroscopic particles in the respiratory tract of humans and rats.

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Michael Fischer, Dipl.-Geoökol.
Helmholtz Zentrum München

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Device development and optimisation of a new technology for fast multi-dimensional chemical analysis of thermal processes, with a special focus on consumer application.

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Harald Grabow, Dipl.-Ing.
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Electronic Engineer

Hardware support and maintenance for chemical instrumentation, in particular nuclear magnetic resonance (NMR) spectrometer servicing, including cryogenics (magnet) and pneumatics (sampler).

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**Jana Grabowsky, Dipl.-LMChem.**  
University of Rostock / Helmholtz Zentrum München  
*PhD Student*

Determination of the molecular signature of different carbonaceous fractions, organic (OC) and elemental carbon (EC), evolving during the thermo-optical analysis of combustion and ambient aerosols.

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**Thomas Gröger, Dipl.-Ing.**  
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*Senior Scientist*

Characterisation of complex molecular systems by chromatographic and mass spectrometric techniques. Special focuses are the conceptional research, further development and application of higher dimensional separation techniques.

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**Beate Gruber, Dipl.-LMChem.**  
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**Anja Gummesson**  
University of Rostock  
*Diploma Student*

Analysis of organic compounds in complex gas mixtures with PTR-MS. The aim of this research is the identification and impact of bacterial volatile organic compounds (VOCs) and volatile organic biomarkers in human exhaled air.

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**Dr. Sabine Haack, Dipl.-Chem.**  
University of Rostock  
*Senior Scientist*

Organisation and implementation of lectures, seminars and analytical practical trainings for students of chemistry, agriculture, biotechnology and for teacher trainees. The emphasis is on trace analysis with AAS, ICP and polarography.

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**Romy Hertz, Dipl.-Chem.**  
University of Rostock / Helmholtz Zentrum München  
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Development of a heated microprobe sampling device coupled with photo-ionisation mass spectrometry (REMPI and SPI) that can be applied, for example, for sampling of (semi)volatile compounds within the glow of a cigarette or inside individual coffee beans during roasting.

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**Jasper Nils Hölzer, Dipl.-LMChem.**  
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Development and validation of an analytical system for fast trace detection of security relevant substances based on an ion trap mass spectrometer coupled with an electron beam pumped excimer light source (EBEL) for internal vacuum ultra violet (VUV) single photon ionisation (SPI).

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**Evelyn Hübner, Dipl.-Ing. (FH)**  
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*Engineer*

Quantification of health-relevant substances in aerosols with GC, HPLC- and LC-MS/MS. Development of chromatographic methods for the identification and determination of organic compounds in environmental and biological matrices.

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**Dr. Gert Jakobi, Dipl.-Chem.**  
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*Scientist*

Monitoring of organic and inorganic compounds in ambient air and deposition; experimental studies concerning their substance inputs in ecosystems. Monitoring of all relevant meteorological parameters.

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**Erwin Karg, Dipl.-Met.**  
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Characterisation of particulate and gaseous atmospheric components; characterisation of particle surface area; experimental aerosol production, instrumentation and analysis; impact of particulates on human health.

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**Kristian Kiersch, Dipl.-Chem.**  
University of Rostock  
*PhD Student*

Development of an analytical system for the determination of pyrolysed organic matter in soil via mass spectrometry (MS) using soft ionisation techniques (field ionisation – FI and photo ionisation - REMPI and SPI).

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Management of environmental studies in Central Europe and the Mediterranean. Monitoring of inorganic/organic compounds in ambient air and deposition in the vicinity of roads/other sources and in remote areas. Performance of studies regarding climate change in the Alps.

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Juliane Kleeblatt, Dipl.-Chem.
University of Rostock / Rostock University Hospital

PhD Student

Direct detection of trace substances in breath gas using Photon Ionisation Mass Spectrometry [Single Photon Ionisation (SPI)-MS and Resonance Enhanced Multiphoton Ionisation (REMPI)-MS].

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Monitoring of hazardous chemical compounds in the environment with special emphasis on POPs in high alpine altitudes.

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Secretary

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Characterisation of the main compounds which cause deposits in diesel engines and to understand their formation mechanism.

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Identification and quantification of relevant constituents of PM, differentiation of the sources of secondary (SOA) and primary (POA) organic aerosols.

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Dr. Jutta Lintelmann, Dipl.-Chem.
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Senior Scientist

Quantification of health-relevant substances in aerosols with HPLC and LC-MS/MS. Development of chromatographic methods for the identification and determination of organic compounds in environmental and biological matrices.

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Helmholtz Zentrum München

Phd Student

Metabolic characterisation of different phases of type 2 diabetes by means of plasma and tissue samples of different mouse models. Integrative examination of the yielded dataset in relation with phenotypical and proteomic data of the same sample material.

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Dr. Jürgen Maguhn, Dipl.-Chem.
Helmholtz Zentrum München

Senior Scientist

Characterisation of ambient aerosol by physical and chemical analysis employing on-line particle counters, impactor probing and aerosol mass spectrometry (AMS).

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Dr. Konrad L. Maier, Dipl.-Biochem.
Helmholtz Zentrum München

Associated Consultant

Radicals in particles: oxidative and proteolytic mechanisms, induction of inflammatory reactions by aerosols.

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Dr. Georg Matuschek, Dipl.-Chem.
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Senior Scientist

Development of personal sampling techniques for the organic-chemical characterisation of environmental aerosols. Quantification of selected targets in model and environmental aerosols of different origins by GC-MS and DTD-GC-MS.

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Makhosazana Mthembu, M.Sc.
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Characterisation of products of coal pyrolysis and Fischer-Tropsch process. The latter is investigated in a homebuilt laboratory reactor.

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Jürgen Orasche, Dipl.-Chem.
University of Göttingen / Helmholtz Zentrum München
PhD Student
Comparison and assessment of stoves, boilers and plants fired by wood combustion as a module for sustainable and renewable generation of energy. Investigations are carried out on the analyses and characterisation of organic tracers in emissions and their behaviour in the environment.
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Markus Oster, Dipl.-Chem.
Helmholtz Zentrum München
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Development of an improved inlet system for laser based single particle aerosol mass spectrometry using soft photo ionisation (REMPI) for selective detection of polycyclic aromatic hydrocarbons.
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Stefan Otto, Dipl.-Chem.
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Characterisation of organic compounds in different environmental compartments, e.g. terrestrial dissolved organic matter in the Baltic Sea, using Pyrolysis-GC, Pyrolysis-MS, Pyrolysis-GC-MS and Pyrolysis-GCxMS analytical techniques. These techniques involve hard and soft ionisation methods.
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Hermann Nordsiek, Dipl.-Chem.
bifa Umweltinstitut GmbH
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Material flow analysis and energy balances in conjunction with dispersion models are tools used for assessment of environmental impact of industrial emissions and consulting on emission control technology. Research on aerosols kinetics at workplace and in thermal processes.
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Analysis and evaluation of analytical data. Analysis of relations between analytical data or data and external sample or sampling parameters.

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Raeed Megeed Qadir, M.Sc.
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Development and application of analytical methods for the characterisation of organic constituents of ambient particulate matter within and outside low emission zones related to health effects.

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Christian Radischat, Dipl.-Chem.
University of Rostock

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On-line and real-time analysis of organic combustion products and trace components in the exhaust gases from fuel/biofuel-powered vehicles and in exhaust gases formed during the combustion of wood. Experiments are carried out with SPI / REMPI-TOF-MS.

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Ahmed Reda, M.Sc.
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Identification and quantification of reactive (semi) volatile organic compounds ((S)VOCs) in emission aerosol in terms of oxygen content.

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Jan Rittgen, Dipl.-Chem.
Federal Criminal Police Office / University of Rostock
PhD Student

Development of lab-based analytical reference procedures, specially contactless and direct MS-techniques for the detection of hazardous materials (explosives, synthetic drugs).

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Organisation and realisation of analytical practical courses. Planning and supervision of experiments.

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Marion Schäffer, M.Sc.
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PhD Student

Development of analytical methods for the chemical characterisation of illicit and pharmaceutical drug samples under forensic aspects based on comprehensive two-dimensional gas chromatography mass spectrometry (GC×GC-TOFMS).

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Phone: +49 (0)89 3187-4239
Claudia Schepler, Dipl.-Chem.
University of Rostock / Helmholtz Zentrum München

PhD Student

Design, construction and characterisation of coupling techniques to combine liquid-chromatography and mass spectrometry using photoionisation. Application for the molecular characterisation of complex samples, such as mineral oils.

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Dr. Jürgen Schnelle-Kreis, Dipl.-Chem.
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Investigation of the impact of aerosols on human health. Chemical characterisation of source and ambient aerosols and source apportionment of ambient aerosols.

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Theo Schwemer
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Diploma Student

Mass spectrometry with soft ionization.

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Dr. Martin Sklorz, Dipl.-Geoökol.
University of Rostock

Senior Scientist

Development of analytical methods and tools basing on mass spectrometry. Special interest in high resolution mass spectrometry, photoionisation sources and coupling techniques to chromatography for getting a deeper insight in environmental and biological processes.

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Dr. Thorsten Streibel, Dipl.-Chem.
University of Rostock

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Improving the comprehension of the formation of organic trace compounds originated from thermal processes such as pyrolysis and combustion. Investigation of the thermal behaviour and characterisation of fossil and regenerative fuels.

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Aimée Celestè Sutherland, M.Sc.
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Development and application of multidimensional comprehensive analysis methods for the investigation of chemical signatures in samples which are relevant for Fischer-Tropsch fuel synthesis.

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Sebastian Wohlfahrt, M.Sc.
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PhD Student

Development of a new technology based on Thermal Analysis (TA), fast gas chromatographic methods (fast-GC) and Time-of-Flight mass spectrometry (ToF-MS) using Electron Impact and Single-Photon Ionization (EI, SPI).

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Anita Wüst
Helmholtz Zentrum München
Technician

Sampling, sample preparation and GC/MS-analyses of target components in aerosols. Routine analysis of health relevant organic substances in environmental samples. Technical support of GC/MS- and DTD-GC/MS-systems.

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Prof. Dr. Ralf Zimmermann, Dipl.-Chem.
University of Rostock / Helmholtz Zentrum München

- Professor of Analytical Chemistry
- Head of the Cooperation Group Comprehensive Molecular Analytics (CMA)
- Head of Joint Mass Spectrometry Centre (JMSC)
- Spokesperson of the Helmholtz Virtual Institute of Complex Molecular Systems in Environmental Health (HICE)

Research Interests

Main research interests include mass spectrometry and in particular photoionisation mass spectrometry, general organic analysis, comprehensive multidimensional separation, environmental and health related research, such as aerosols.

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www.jmsc.de
www.hice-vi.eu
Funding and Scholarships
<table>
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<th>Nr</th>
<th>Source / Project</th>
<th>Period</th>
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<td>Bavarian State Ministry of the Environment and Public Health/Technische Universität München (BSfMUG/TUM) Auswirkungen des Klimawandels in den Alpen – Erfassung mittels Höhengradienten</td>
<td>08-12</td>
<td>30,900</td>
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<td>2</td>
<td>University of Göttingen Nachhaltige Nutzung von Energie aus Biomasse im Spannungsfeld von Klimaschutz, Landschaft und Gesellschaft – TP Schadstoffemissionen bei der Energiewinnung aus Stroh, Holz und Biogas</td>
<td>09-14</td>
<td>118,782</td>
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<td>3</td>
<td>German Social Accident Insurance (DGUV) Untersuchung der Messfehler bei der Probenahme von Gefahrstoff-Aerosolen in Arbeitsbereichen (Messfehler Aerosole)</td>
<td>10-13</td>
<td>403,706</td>
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<td>German Federal Criminal Police Office (BKA) Neue Wege des Impurity-Profilings von Arzneimitteln, Dopingsubstanzen und biogenen Drogen mittels zweidimensionaler Gaschromatographie</td>
<td>11-12</td>
<td>29,906</td>
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<td>Initiative and Networking Fund of the Helmholtz Association (IVF) – VH-VI-418 Helmholtz Virtual Institute of Complex Molecular Systems in Environmental Health (HICE)</td>
<td>12-16</td>
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<td>Bavarian Environment Agency (LfU) Erfassung von POP im Alpenraum</td>
<td>08-11</td>
<td>75,600</td>
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<td>7</td>
<td>Federal Ministry of Education and Research (BMBF), VDI Technologiezentrum GmbH Verbundprojekt: Detektion von sicherheitsrelevanten Substanzen in schwer zugänglichen Orten (SAFE INSIFE) – Teilvorhaben: Grundlegende Anpassung des Ionenfallen-Massenspektrometers</td>
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<td>Land Salzburg/European Regional Development Fund CO2-NeuTrAlp – CO2-neutral transport for the Alpine Space</td>
<td>08-12</td>
<td>109,989</td>
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<td>Bayerische Forschungsstiftung/ Netzsch-Gerätebau GmbH Mehrdimensionale Analyse thermischer Prozesse</td>
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* UR and HMGU Funding.
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<td>10</td>
<td>DFG / ZI 764/3-1 Entwicklung und Anwendung eines gekoppelten Thermodesorption/Photoionisations-Massenspektrometers für die Bestimmung der Beschaffenheit der kohlenstoffhaltigen Fraktion des oligomeren/polymeren Gehalts von Umweltaerosol</td>
<td>08-11</td>
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<td>11</td>
<td>Netzsch Gerätebau GmbH TG-Skimmer-MS: Charakterisierung und Optimierung der Jet-Eigenschaften</td>
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<td>Sasol (Pty) Ltd. Application of REMPI-/SPI-TOFMS für on-line analysis of coal pyrolysis products and Fischer-Tropsch micro reactor streams</td>
<td>08-12</td>
<td>178,500</td>
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<td>13</td>
<td>Wissenschaftsgemeinschaft Gottfried Wilhelm Leibnitz e.V Abbaubarkeit von aktischen, terrigenem Kohlenstoff im Meer“ (ATKiM)</td>
<td>11-14</td>
<td>135,700</td>
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<td>15</td>
<td>BAT Cigarette Combustion Projects</td>
<td>10-13</td>
<td>225,672</td>
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<td>16</td>
<td>Sasol (Pty) Ltd Development of multidimensional analysis methods for investigation of Coal Gasification and Fischer-Tropsch synthesis</td>
<td>11-15</td>
<td>233,240</td>
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</table>

**Total funding sum:** EUR 6,067,045
## PhD Scholarships

<table>
<thead>
<tr>
<th>Name</th>
<th>Institution</th>
<th>Source</th>
<th>Period</th>
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<tbody>
<tr>
<td>Juliane Kleeblatt</td>
<td>University of Rostock, Interdisciplinary Faculty</td>
<td>Dept. of Life, Light and Matter, University of Rostock</td>
<td>09-12</td>
</tr>
<tr>
<td>Fengxia Li</td>
<td>Peking University, China</td>
<td>Chinese Scholarship Council (CSC)</td>
<td>11-15</td>
</tr>
<tr>
<td>Makhosazana Mthembu</td>
<td>Sasol (Pty) Ltd., South Africa</td>
<td>Sasol (Pty) Ltd.</td>
<td>08-13</td>
</tr>
<tr>
<td>Raeed Qadir</td>
<td>University of Duhok, Dept. of Chemistry, College of Science, Irak</td>
<td>German Academic Exchange Service (DAAD)</td>
<td>10-12</td>
</tr>
<tr>
<td>Ahmed Reda</td>
<td>Al-Nahrain University, Baghdad, Irak</td>
<td>German Academic Exchange Service (DAAD)</td>
<td>11-12</td>
</tr>
<tr>
<td>Sevinj Sadigova</td>
<td>Baku State University, Azerbaijan</td>
<td>German Academic Exchange Service (DAAD)</td>
<td>10/11-12/11</td>
</tr>
<tr>
<td>Claudia Schepler</td>
<td>University of Rostock</td>
<td>Landesgraduierten-stipendium</td>
<td>10-12</td>
</tr>
<tr>
<td>Aimée Sutherland</td>
<td>Stellenbosch University, South Africa</td>
<td>Sasol (Pty) Ltd.</td>
<td>12-15</td>
</tr>
</tbody>
</table>
Teaching and Conference Participation
Mass Spectrometry Seminars

The Mass Spectrometry Seminar (MS Seminar) is held each semester at the University of Rostock (Chemistry Main Building, SR 01, 5:30 pm) and is viewed via skype by members and guests of the CMA at Helmholtz Zentrum München.

SUMMER TERM 2011

12.04.2011 . Prof. Dr. U. Karst
Univ. of Münster
GDCh Fresenius Lecture: Analytische Kopplungstechniken: Leistungsstarke Werkzeuge zur Lösung biomedizinischer Fragestellungen

26.04.2011 . Dr. K. Dettmer
Univ. of Regensburg
Strategien zur analytischen Bezwingung des Metabolomics Eisberges

10.05.2011 . Prof. Dr. M. Linscheid
HU Berlin
Metallmarkierung zur Quantifizierung von Biopolymeren

17.05.2011 . Dr. T. Dittmar
Univ. of Oldenburg
Ultrahochauflösende Massenspektrometrie (FT-ICR-MS) in der Meeresforschung

31.05.2011 . Dr. T. Möhring
Thermo GmbH, Bremen/Germany
Theory and Practice of the Orbitrap Mass Analyzer

14.06.2011 . Dr. A. Ingendoh
Bruker-Daltonics GmbH, Bremen/Germany
FTMS - Überblick neuerer Entwicklungen und Anwendungen

21.06.2011 . Dipl.-Chem. S. Eichholz
Netzsch GmbH, Selb/Germany
Gasanalytische Kopplungsmethoden der Thermischen Analyse

28.06.2011 . Dr. O. Jahn, PhD
MPI Göttingen
Characterization of Biomolecular Interactions by Photoaffinity Labeling and Mass Spectrometry: The Munc13/Calmodulin Complex

05.07.2011 . Prof. Dr. W. Weinmann
Univ. of Bern/Switzerland
LC-MS/MS in der Forensischen Toxikologie und Alkoholismus-Diagnostik

12.07.2011 . Prof. Dr. Th. Benter
Univ. of Wuppertal
Atmospheric Pressure Ionization: What Do We Really Know?
WINTER TERM 2011/2012

18.10.2011 • Prof. Dr. R. Nießner
TU München
GDCh Fresenius Lecture: Laser oder Antikörper - Zwei Freunde des Analytikers

01.11.2011 • Dr. B. Linden
Linden CMS GmbH
LIFDI - Eine Universelle Ionisierungstechnik für Diffizile Substanzen

07.11.2011 • Nano SIMS Workshop am IOW
Vorträge im Rahmen des Nano SIMS Eröffnungs-Workshop am IOW

08.11.2011 • Dr. D. Schaumlöffel CNRS/Université de Pau et des Pays de l'Adour, France
Die Element-Massenspektrometrie in der Bioanalytik: ICP-MS zur Dektektion und Quantifizierung von Biomolekülen

15.11.2011 • Dr. J. Wendt
LECO Instruments
Time-of-Flight taking off - Technik und Anwendung

22.11.2011 • Prof. Dr. L. Mondello, Prof. Dr. P. Tranchida
Univ. of Messina, Italy
A Novel Flow Modulator for Comprehensive 2D GC (L. Mondello)
Rapid Elucidation of Hydrocarbon Contamination in Foods by Using Multidimensional LC-GC (P. Tranchida)

29.11.2011 • Prof. M. Glocker
Univ. of Rostock
Are There Really Applicable Protocols Suitable for MALDI-MS-Based Phosphopeptide Stability Estimations?

13.12.2011 • Dr. M. Gonin
TOFWERK AG, Thun
Flugzeugmassenspektrometer - Prinzip, Aufbau, Datenerfassung und Anwendungen

10.01.2012 • Dr. W. Schrader
MPI für Kohleforschung
Impact of Analytical Chemistry on Energy Research: From Ultra-High Resolution to Sample Simplification

17.01.2012 • Prof. Dr. J. Broekaert
Univ. of Hamburg
Possibilities and Limitations of New Ion Sources for the Mass Spectrometric Determination of the Elements and their Compounds
Lectures, Practical Courses and Seminars

The following were courses held at the Chair of Analytical Chemistry during the Academic Year 2011-2012.

**LECTURES**

**Summer Term 2011 • Principles of Analytical Chemistry (2 SWS)**
Compulsory Lecture for Chemists
*PD Dr. G.-U. Flechsig*

**Summer Term 2011 • Instrumental Analytical Chemistry I (4 SWS)**
Compulsory Lecture for Chemists
*Prof. Dr. R. Zimmermann*

**Summer Term 2011 • Analytical Chemistry (1 SWS)**
Compulsory Lecture for Medical Biotechnologists
*Dr. S. Haack*

**Summer Term 2011 • Analytical Chemistry (1 SWS)**
Compulsory Lectures for Chemists (Teacher Training Course)
*Prof. Dr. R. Zimmermann*

**Summer Term 2011 • Analytical Chemistry II - Environmental Analytics (2 SWS)**
Compulsory Lectures for Chemists
*Prof. Dr. R. Zimmermann*

**Winter Term 2011/2012 • Analytical Chemistry III/TCII Instrumental Analytics of Biotechnology (2 SWS)**
*Prof. Dr. Ralf Zimmermann*

**Winter Term 2011/2012 • Analytical Chemistry V: Modern Methods of Mass Spectrometry and Chromatography (2 SWS)**
*Prof. Dr. Ralf Zimmermann*

**PRACTICAL COURSES**

**Summer Term 2011 • Analytical-Chemical Practical Course (1 SWS)**
Compulsory for Medical Biotechnology

**Summer Term 2011 • Practical Course in Instrumental Analytics (4 SWS)**

**Summer Term 2011 • Practical Course in Area of Specialization (12 SWS)**
Advanced Lab Course for Chemists

**Summer Term 2011 • Environmental Chemistry (3 SWS)**
Compulsory Lab Course for Chemists (Teacher Training Course)

**Winter Term 2011/2012 • Analytical-Chemical Lab Course (1 SWS)**
Compulsory for Agricultural Ecologists
**Winter Term 2011/2012 • Methods in Analytical Chemistry**  
Compulsory Lab Course for Chemists

**Winter Term 2011/2012 • Analytical Chemistry - Basics**  
Compulsory Lab Course for Chemists

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**SEMINARS**

**Summer Term 2011 • Principles of Analytical Chemistry (2 SWS)**  
Optional for Chemists  
*PD Dr. G.-U. Flechsig*

**Summer Term 2011 • Analytical Chemistry II - Environmental Chemistry (1 SWS)**  
*Dr. T. Streibel*

**Winter Term 2011/2012 • Analytical Chemistry III/TCII Instrumental Analytics of Biotechnology (2 SWS)**

*Prof. Dr. Ralf Zimmermann*

**Winter Term 2011/2012 • Analytical Chemistry V: Modern Methods of Mass Spectrometry and Chromatography (2 SWS)**

*Prof. Dr. Ralf Zimmermann*

**Summer Term 2011 and Winter Term 2011/2012 • Analysis of Complex Molecular Systems (1 SWS)**  
Research Seminar for Master and PhD Students  
*Prof. Dr. R. Zimmermann*

**Summer Term 2011 and Winter Term 2011/2012 • Seminar of the Mass Spectrometry Centre (1 SWS)**  
Interdisciplinary Seminar: New Methods of Mass Spectrometry and Chromatography  
*Prof. Dr. R. Zimmermann and Invited Guest Scientists*

**Summer Term 2011 and Winter Term 2011/2012 • Modern Instrumental Analytics (1 SWS)**  
Research Seminar for Master and PhD Students  
*Prof. Dr. R. Zimmermann*
Lectures at National and International Conferences 2011/2012

The following is a list of lectures delivered at national and international conferences/workshops sorted by date.

**March 21, 2012** • R. Zimmermann, T. Streibel, M. Sklorz
*Photoionisations-Massenspektrometrie mit Lasern und inkohärenten Lichtquellen*
University of Innsbruck, Austria, Invited Seminar Lecture (fully funded)

**March 11-15, 2012** • S. Ehlert, J. Hölzer, M. Sklorz, A. Walte, M. Pütz, R. Zimmermann
*Laser-Desorption for Real-Time Detection of security relevant substances at ambient conditions*
Pittcon 2012 - Pittsburgh Conference on Analytical Chemistry and Applied Spectroscopy, Orlando, Florida, USA

**March 11-16, 2012** • P. Trefz, J. K. Schubert, D. Hein, W. Miekisch
*Micro extraction techniques as a link between clinical application and hyphenated analytical techniques*
Pittcon 2012 - Pittsburgh Conference on Analytical Chemistry and Applied Spectroscopy, Orlando, Florida, USA

**March 11-15, 2012** • R. Zimmermann, M. S. Eschner, T. Gröger, M. Gonin
*Rapid switching (80 Hz) between hard electron ionization (EI) and soft photo ionization (SPI) for gas chromatography/time-off-flight mass spectrometry: Technical realization and applications*
Joint Conference of the German Mass Spectrometry Society (DGMS) and the Polish Mass Spectrometry Society, Poznań, Poland

**February 9, 2012** • R. Zimmermann, T. Streibel, R. Hertz, M. Sklorz, A. Fendt, M. Oster
*Photo ionization mass spectrometry for organic profiling*
University of Oviedo, Spain, Invited Seminar Lecture (fully funded)

**February 1-3, 2012** • R. Zimmermann, T. Gröger, S. Ly-Verdu, M. Eschner
*Multidimensional analysis for metabolomics: Application of GC and GCxGC coupled to mass spectrometry with soft or hard ionization*
12th HTC-Symposium, Bruges, Belgium, Invited Royal Chemical Society Seminar Lecture (partially funded)
Organische Emissionen bei der Verbrennung von Holz, Stroh und Biogas, Fachtagung Chancen und Risiken der Bioenergie im Kontext einer nachhaltigen Entwicklung
Fachtagung Chancen und Risiken der Bioenergie im Kontext einer nachhaltigen Entwicklung, Göttingen, Germany

New concepts for on-line monitoring of complex gas mixtures using photo ionization mass spectrometry
XVIII SASP 2012– Alpe d’Huez, France

Organische Verbindungen in Aerosolen – Eine Herausforderung für die chemische Analytik
Institute for Meteorology and Climate Research, Atmospheric Aerosol Research, KIT, Invited Seminar Lecture (fully funded)

Photo ionization mass spectrometry: New concepts and applications ATC, SASOL Analytical Conference, Johannesburg, South Africa

Organic compounds in ambient aerosols: Sources and health effects University of KwaZulu-Natal, South Africa, Invited Seminar Lecture (fully funded)

Charakterisierung von Biomassepyrolyse und Kraftstoffen mit online-Massenspektrometrie und zweidimensionaler Gaschromatographie
5. Rostocker Bioenergieforum 2011, Rostock, Germany

Photo ionization mass spectrometry for on-line characterizations of industrial and technical combustion and pyrolysis processes
14th BECIA, Beijing, China, Invited Lecture (fully funded)

Spatial and temporal variability of biomass burning organic aerosol in Augsburg, Germany
AAAR Conference 2011, Orlando, Florida

October 2-6, 2011 • T. Streibel, C. Busch, C. Radischat, R. Zimmermann
Resonance enhanced multi-photon ionization time-of-flight mass spectrometry for monitoring the pattern and dynamic behaviour of polyaromatic compounds in combustion and pyrolysis off-gases from solid fuels
FACSS 38th Annual Meeting 2011, Reno, Nevada, USA

October 2-6, 2011 • J. Grabowsky, T. Streibel, M. Sklorz, R. Zimmermann
Photo-ionization time-of-flight mass spectrometry coupled to a carbon analyzer to investigate the organic content of carbon fractions from particulate matter
FACSS 38th Annual Meeting 2011, Reno, Nevada, USA
September 18-21, 2011 • R. Zimmermann, M. Eschner, M. Bente, M. Saraji, A. Walte
Detection of the molecular composition of pyrolysis gases in thermal analysis (TA) using photo ionization TOF MS for evolved Gas Analysis (EGA): Instrumental set-up and first results on tobacco and cigarette materials
TSRC 2010, Lexington, KY, USA

September 18-21, 2011 • R. Zimmermann, N. Rose, A. Walte, M. Bente, M. Saraji, M. Eschner, T. Gröger
Puff-resolved on-line real-time analysis and quantification of tobacco smoke components by a commercial smoke profiler/Smoking machine - Photo Ionisation TOF-Mass Spectrometer system
TSRC 2010, Lexington, KY, USA

September 4-8, 2011 • T. Streibel, C. Busch, C. Radischat, K. Mthembu, R. Zimmermann
Resonance enhanced multi-photon ionization time-of-flight mass spectrometry for monitoring the pattern and dynamic behaviour of polyaromatic compounds in combustion and pyrolysis off-gases from solid fuels
23rd International Symposium on Polycyclic Aromatic Compounds, ISPAC 23, Münster, Germany

Hourly concentrations of organic tracers originated from wood combustion
EAC, Manchester, UK

September 4-9, 2011 • J. Schnelle-Kreis, J. Gu, G. Abbaszade, J. Diemer, R. Zimmermann
Spatial distribution of ambient particulate matter and source contributions in Augsburg, Germany
EAC, Manchester, UK

September 4-9, 2011 • R. Zimmermann, Ch. Deuerling, R. Warnecke, H. Nordsieck, J. Maguhn, F. Mühlberger, T. Streibel
On-line measurement of chemical composition and size distribution of high-temperature combustion aerosol
EAC, Manchester, UK

August 28 - September 2, 2011 • R. Zimmermann, T. Streibel, R. Hertz, A. Fendt, M. Sklorz, M. Eschner, M. Bente, M. Oster, A. Walte
Photo-ionisation mass spectrometry for on-line analysis: Monitoring of the coffee roasting process, real-time analysis of cigarette smoke and other applications
XXXVIII Colloquium Spectroscopicum Internationale (CSI), Buzios, Brazil, Invited Key Note Lecture (partially funded)

August 28 - September 2, 2011 • R. Zimmermann, M. Eschner, T. Gröger, M. Gonin
Multidimensional comprehensive separation by gas chromatography (GC) coupled to a soft photo ionization mass spectrometer: Simultaneous recording of hard electron ionization and soft photo ionization mass spectra
XXXVIII Colloquium Spectroscopicum Internationale (CSI), Buzios, Brazil (partially funded)

July 7, 2011 • R. Zimmermann, M. Eschner, T. Gröger, W. Welthagen
Multidimensional comprehensive separation by GC-MS and GCxGC-MS: Simultaneous recording of hard and soft mass spectra and multidimensional separation space
Seminar at University of Messina, Messina, Italy, Invited Lecture (fully funded)
June 30, 2011 • M. Kirchner and G. Jakobi
International Conference: On the Road to Sustainable Mobility: Where Are We Going?
Milan, Italy

Institute of Ecological Chemistry and its succeeding research units: The Cooperation Group “Comprehensive Molecular Analytics” – CMA and the “Joint Mass Spectrometric Centre” – JMSC
MidTerm Review at the Helmholtz Zentrum München, Munich, Germany

In-Situ Derivatization Thermal Desorption (IDTD) GC-TOF MS for characterization of wood combustion sources
10th International Conference on Carbonaceous Particles in the Atmosphere (ICCPA) 2011, Vienna, Austria

Berlin, Germany

June 6-10, 2011 • T. Streibel
Mass spectrometry applying soft photo-ionisation for real time characterisation of transients from flash pyrolysis of biomass
Workshop at 19th European Biomass Conference and Exhibition, Berlin, Germany

June 8, 2011 • R. Zimmermann, J. Schnelle-Kreis, J. Orasche, M. Oster, M. Elsasser
Analysis of wood combustion aerosols in ambient air using inorganic and organic tracer compounds
12th International Congress on Combustion By-Products and their Health
E (PIC-Congress), Hangzhou, China

June 8, 2011 • R. Zimmermann, T. Streibel, A. Fendt, M. Sklorz, M. Eschner, M. Bente, A. Walte
Photo ionisation mass spectrometry for on-line characterisation of industrial and technical combustion and pyrolysis processes
12th International Congress on Combustion By-Products and their Health
E (PIC-Congress), Hangzhou, China

Aplication of thermal desorption-GC-MS in the analysis of particulate organic matter
3rd Sino-German Workshop on Aerosols and Health, Lanzhou, China

Analysis of organic compounds in ambient and source particulate matter
3rd Sino-German Workshop on Aerosols and Health, Lanzhou, China

Soft Photo-Ionisation Mass Spectrometry for analysis of complex organic mixtures: New concepts and applications
ICAS, Kyoto, Japan, May 2011, Invited Lecture (fully funded)
May 6, 2011 • R. Zimmermann, J. Grabowski, T. Streibel, M. Sklorz
Coupling of REMPI-/SPI-TOFMS gas analyzer to the DRI EC/OC Instrument: Progress report
Seminar at the Desert Research Institute, Reno, NV, USA

May 1-5, 2011 • R. Zimmermann, M. Eschner, T. Gröger, M. Gonin
Multidimensional comprehensive separation by GC-TOFMS and GCxGC-TOFMS with simultaneous recording of hard electron ionization and soft photo ionization mass spectra: Technical realization and applications
ISCCE & GCxGC 2011, San Diego, CA, USA, Invited Lecture (fully funded)
Publications
The following are publications of the reporting period 04/2011 - 03/2012.

Application of modern online instrumentation for chemical analysis of gas and particulate phases of exhaust at the European Commission Heavy-Duty Vehicle Emission Laboratory

S. Dresen, S. Kneisel, W. Weinmann, R. Zimmermann and V. Auwaerter
Development and validation of a liquid chromatography-tandem mass spectrometry method for the quantitation of synthetic cannabinoids of the aminoalkylindole type and methanandamide in serum and its application to forensic samples

Ambient PM(10) concentrations from wood combustion - Emission modeling and dispersion calculation for the city area of Augsburg, Germany

Online characterization of regulated and unregulated gaseous and particulate exhaust emissions from two-stroke mopeds: A chemometric approach
Original Research Article
Analytica Chimica Acta, Volume 717, 2 March 2012, p. 28-38

T. Eickner, S. Mikkat, P. Lorenz, M. Sklorz, R. Zimmermann, H.-J. Thiesen and M. O. Glocker
Systematic studies on TiO2-based phosphopeptide enrichment procedures upon in-solution and in-gel digestion of proteins: Are there readily applicable protocols suitable for matrix-assisted laser desorption/ionization mass spectrometry based phosphopeptide stability estimations?
M. S. Eschner and R. Zimmermann
Determination of photoionization cross-sections of different organic molecules using gas chromatography coupled to single-photon ionization (SPI) time-of-flight mass spectrometry (TOF-MS) with an electron-beam-pumped rare gas excimer light source (EBEL): Influence of molecular structure and analytical implications

T. M. Groeger and R. Zimmermann,
Online comprehensive two-dimensional characterization of puff-by-puff resolved cigarette smoke by hyphenation of fast gas chromatography to single-photon ionization time-of-flight mass spectrometry: Quantification of hazardous volatile organic compounds

M. S. Eschner, T. M. Groeger, T. Horvath, M. Gonin and R. Zimmermann
Quasi-simultaneous acquisition of hard electron ionization and soft single-photon ionization mass spectra during GC/MS analysis by rapid switching between both ionization methods: Analytical concept, setup, and application on diesel fuel

Hyphenation of a carbon analyzer to photo-ionization mass spectrometry to unravel the organic composition of particulate matter on a molecular level

T. M. Groeger and R. Zimmermann,
Application of parallel computing to speed up chemometrics for GC x GC-TOFMS based metabolic fingerprinting

T. M. Groeger, S. Nathoob, T. Kub, S. Sikorab, R. J. Turner and E. J. Prenger
Real-time imaging of lipid domains and distinct coexisting membrane protein clusters

Source apportionment of ambient particles: Comparison of positive matrix factorization analysis applied to particle size distribution and chemical composition data

R. Hertz, T. Streibel, C. Liu, K. McAdam and R. Zimmermann
Microprobe sampling-photo ionization-time-of-flight mass spectrometry for in situ chemical analysis of pyrolysis and
combustion gases: Examination of the thermo-chemical processes within a burning cigarette
*Original Research Article Analytica Chimica Acta*, Volume 714, 10 February 2012, Pages 104-113


Particle-associated organic compounds and symptoms in myocardial infarction survivors
*Inhalation Toxicology*, 2011. 23(7): p. 431-447


The dynamic range of the human metabolome revealed by challenges


In-situ derivatization thermal desorption GC-TOFMS for direct analysis of particle-bound non-polar and polar organic species
*Atmospheric Chemistry and Physics Discussions*, 2011. 11: p. 15255-15295


Technical Note: In-situ derivatization thermal desorption GC-TOFMS for direct analysis of particle-bound non-polar and polar organic species
*Atmospheric Chemistry and Physics*, 11, 8977-8993, 2011. doi: 10.5194/acp-11-8977-2011

M. Oster, M. Elsasser, J. Schnelle-Kreis and R. Zimmermann

First field application of a thermal desorption resonance enhanced multiphoton ionisation single particle time-of-flight mass spectrometer for the online detection of particle bound polycyclic aromatic hydrocarbons in Augsburg, Germany in winter 2010
*Analytical and Bioanalytical Chemistry*, 2011. 401: p. 3153–3164


Seasonal variation and source estimation of organic compounds in urban aerosol of Augsburg, Germany


Detection of organic products of polymer pyrolysis by thermogravimetry-supersonic jet-skimmer time-of-flight mass spectrometry (TG-Skimmer-SPI-TOFMS) using an electron beam pumped rare gas excimer VUV-light source (EBEL) for soft photo ionisation


Investigation of polymers by a novel analytical approach for evolved gas analysis in thermogravimetry

Influences of the 2010 Eyjafjallajökull volcanic plume on air quality in the northern Alpine region
Atmos Chem Phys, 2011. 11: 8555-8575

M. Schäffer, T. M. Groeger, M. Pütz, S. Dieckmann and R. Zimmermann
Comparative analysis of the chemical profiles of 3,4-methylenedioxy-methamphetamine based on comprehensive two-dimensional gas chromatography time-of-flight mass spectrometry (GC×GC-TOFMS)
Journal of Forensic Sciences, in press

Application of direct thermal desorption gas chromatography time-of-flight mass spectrometry for determination of non-polar organics in low volume samples from ambient particulate matter and personal samplers

Phase-resolved real-time breath analysis during exercise by means of smart processing of PTR-MS data

P. Trefz, S. Kischkel, D. Hein, E. S. James, J. K. Schubert and W. Miekisch
Needle trap micro-extraction for VOC analysis: Effects of packing materials and desorption parameters
Helmholtz Virtual Institute
HICE
Dear Reader,

In addition to the annual report of the Joint Mass Spectrometry Centre of the University of Rostock and the Helmholtz Zentrum München (JMSC) you will find in the following section a description of the research outline and structure of the newly founded Helmholtz Virtual Institute of Complex Molecular Systems in Environmental Health – Aerosol and Health (HICE). The basic idea of HICE is to bring together aerosol science and physics, high-end chemical and molecular biology analytics, toxicologists as well as engineers and - in a later stage - animal tests and clinical researchers, in order to elucidate the primary biological and health effects of aerosols from anthropogenic sources in a comprehensive and interdisciplinary manner.

HICE was proposed by the JMSC in early 2011 to the Helmholtz Association (HGF). After a competitive peer-review evaluation of the written proposal as well as an oral proposal defence hearing by a delegation of the HICE consortium in June 2011 in front of an expert committee headed by the HGF president Prof. Mlynek at the HGF headquarters in Berlin, the proposal was eventually accepted in October 2011. The granting period of 5 years (3 + 2 years with an evaluation after the first 3 years) started on January 1st 2012.

In addition to the JMSC, further research groups at University of Rostock (UR), Helmholtz Zentrum München (HMGU), the Technische Universität München (TUM), the Max Delbrück Centre of Molecular Medicine (MDC), the Karlsruhe Institute of Technology (KIT), the University of Luxemburg (ULUX), the University of Eastern Finland (UEF) and the University of Cardiff (UCA) are included in the HICE funding. Furthermore, a variety of industrial and academic partner are associated to HICE.

Personally, I am convinced that we succeeded in building a very strong, sound consortium to address the HICE research questions. The HICE funding, however, needs to be seen as “seed money” and the scientific success of HICE is also contingent on further efforts of the HICE partners to raise additional third party funding for the whole consortium or sub-groups. This also includes further steps towards a more elaborated research structure for the permanent cooperation between the University of Rostock and the Helmholtz Zentrum München.

In the following, the fundamental scientific research program and concept as well as the basic hypotheses of HICE are briefly summarised and the national and international partners are introduced. Finally, I would like to invite the readers of this report to follow the progress of the HICE consortium and its research program as well as the achieved results in the future annual reports of the JMSC & HICE as well as in the scientific literature and congresses.

Prof. Dr. Ralf Zimmermann

Chair of Analytical Chemistry
Head of JMSC
HICE Spokesperson
Aim, Strategic Partnership and Structure of HICE

The "Helmholtz Virtual Institute of Complex Molecular Systems in Environmental Health - Aerosols and Health" (HICE) was founded on January 1, 2012.

HICE comprehends work of research groups from eight partner institutions on health effects of anthropogenic aerosols and is represented by the spokesperson Prof. Dr. Ralf Zimmermann from the Joint Mass Spectrometry Centre (JMSC) of the Helmholtz Zentrum München (HMGU, Cooperation Group “Comprehensive Molecular Analytics”) and the University of Rostock (UR, Chair of Analytical Chemistry). In addition to the eight partners, five associated partners from academia or industry have joined the HICE network. The motivation for the HICE program arises from the observed large effects of air pollution, in particular the concentration of particulate matter (PM), on life expectancy (see Figure 1). In the developed counties, PM actually represents the most severe environmental effect on life expectancy and human health.

Figure 1 | Loss in life expectancy (months) attributable to exposure to fine particulate matter (PM2.5) in 2000. Source: EU-Clean Air For Europe (CAFE).
**Research Aim**

The objective of the HICE is the establishment of a long-term scientific research initiative for the investigation of the causes and mechanisms of environmentally influenced diseases. Within the 5-year funding period, the research program of HICE will focus on a deeper understanding of the impact of anthropogenic aerosols on human health. Based on current hypotheses, reactive organic compounds in particle as well as in gas phase of aerosols are particularly relevant. Innovative in-vitro human lung tissue models are exposed to aerosols and separated gas and particle phases from relevant aerosol sources. The response of the biological systems is investigated by state-of-the-art analytical techniques on different biological levels (transcriptome, proteome, metabolome, and toxicological parameters). A unique approach is the application of novel mass spectrometry-based analytical methods for comprehensive, non-targeted analyses of small molecules in combination with stable isotope labelling approaches for detection of flux changes in the metabolism. The complex biological response data is chemometrically and biostatistically analysed in conjunction with comprehensive chemical and physical data of the aerosol used for exposure in order to identify biomarkers of exposure, harm and disease. Figure 2 depicts the general scheme of the planned research activities in HICE. The main hypotheses to be investigated in HICE are as follows:

![Diagram](image.png)

**Figure 2** | General scheme of the planned research activities in HICE. In the first period (3 years) human lung cells are exposed to aerosols, particles and gases. The biological system is comprehensively characterised before and after exposure. Furthermore, the chemical signature of the aerosols, particles and gases to which the cells are exposed is analysed in detail. All collected data is then jointly analysed by chemometric and biostatistical tools.
Hypothesis 1
"Reactive organic compounds in the emitted or aged aerosols are relevant for observed health effects."

Hypothesis 2
"Synergistic effects of gas phase and the particulate phase organics are important for biological effects and the observed health effects."

Hypothesis 3
"The change to more bio fuel utilization & bio mass combustion will alter the aerosol composition and also health effects."

Hypothesis 4
"The application of cell exposure systems, which allow a defined exposure of lung cells or cell based tissue models at the Air-Liquid-Interface (ALI) in conjunction with a comprehensive metabolomics/proteomics & flux analyses will allow an improved detection of early biological effects in the model systems."

The General Concept of Helmholtz Virtual Institutes
In general, a Helmholtz Virtual Institute shall bring together key competencies of one or more Helmholtz Centres with those of one or more universities to create a centre of excellence of international standing. The Helmholtz Virtual Institutes are co-funded by the Initiative and Networking Fund (INF) of the Helmholtz Association (HGF). Helmholtz Virtual Institutes shall establish and extend research partnerships between Helmholtz Centres and German universities, generate new collaborations with leading international partner institutions and provide a distinct benefit in preparing the way for larger strategic research projects, such as the Helmholtz Alliances and Institutes. In addition, the eligibility of the HICE consortium for additional national and European funding shall be enhanced. With the funding mechanism the Helmholtz Association wants in particular to strengthen the position of universities in the German scientific system.

Strategic Partnership
The Joint Mass Spectrometry Centre (JMSC) of the Helmholtz Zentrum München and the University of Rostock forms a backbone structure within HICE. The analytical and aerosol-physical expertise of the JMSC is complemented by biological, engineering, clinical and toxicological expertise of further institutes of the Helmholtz Zentrum München and the University of Rostock, the Technische Universität München (TUM), the Karlsruhe Institute of Technology (KIT) and the Max Delbrück Center (MDC). Three outstanding international partners, the University of Luxembourg (ULUX), the University of Cardiff (UCA) and the University of Eastern Finland (UEF) as well as associated partners from commercial business (Vitrocell systems GmbH, Photonion GmbH, Decodon GmbH and ASG GmbH) and non-university research institutions (Joint Research Centre, Ispra and the Baltic Sea Research Institute, Warnemünde) complete the expertise profile of HICE. In Figure 3 the eight funded partners are indicated.

Structure and Education
In addition to bringing together complementary techniques, the Virtual Institute implements new organisational structures to ensure the success of different interdisciplinary groups to one interacting institute and to build a long-term structure. This enables the consortium to attract sufficient third-party funds to accomplish the research tasks. The interdisciplinary research of HICE is structured in four well-defined and interrelated work packages with their own leading structure.
Work Package I
In Work Package I the characterisations of relevant organic compounds in aerosols, gases and particulate matter are performed. The central aim of WP I is the characterisation of reactive organic compounds in aerosols with an emphasis on the gas phase. In addition, a large variety of source and model aerosols are provided for exposure experiments.

Work Package II
In Work Package II, the toxicology of organic components in aerosols is addressed. The biological effects of freshly...

Figure 3 | Funded partners of HICE.
generated whole, denuded (i.e. particles only) and “filtered” (i.e. gas phase only) combustion aerosols on human lung cell models (cultured in-vitro at the air-liquid interface) are comparatively investigated. Relevant aerosol sources are investigated, including wood combustion (heating), ship diesel emission and emissions from trucks, gasoline and diesel passenger cars. For the internal combustion engines furthermore the application of bio fuels is addressed (e.g. bio diesel or ethanol). Additionally, the effect of the investigated aerosol sources on animal models shall be studied in a later stage of HICE. Finally, results from in-vitro and in-vivo studies should be transferred to the investigation of human specimen.

Work Package III
In Work Package III (Small Molecules and Isotope Labelling) the comprehensive chemical analysis of molecules and molecular signatures in aerosols and biological systems is performed. WP III focuses on the comprehensive chemical analysis of aerosols as well as the evaluation of changes in the pattern of small molecules (Metabolites) as well as proteins in the biological test systems caused by the impact of aerosols. One aspect is the characterisation of the chemical composition of the different compartments of the aerosol. A second aspect is the investigation of the impact of chemically and physically well characterised aerosols on biological test systems and their potential health effects.
Work Package IV
In Work Package IV (Chemometry and Biostatistics) finally scientific data management, chemometrics and biostatistical approaches to address the complex molecular effects are summarized. WP IV is one central interface within the framework of the HICE. It is responsible for the combined statistical data analysis comprising all

Helmholtz Virtual Institute of Complex Molecular Systems in Environmental Health - HICE

Virtual Institute Scientific Steering Board (VISB)
Spokesperson HICE: Prof. Dr. Ralf Zimmermann (HMGU, UR)
Spokespersons Work Packages:
- Prof. Jorma Jokiniemi (UEF), Dr. Hanns-Rudolf Paur (KIT), Dr. Gunnar Dittmar (MDC), N.N.

Virtual Institute Management and Administration (VIMA)
Project Management: Sorana Scholtes

Work Package I
Aerosol Characterisation
WP Spokespersons
1. Prof. Jorma Jokiniemi (UEF)
2. Dr. T. Streibel (UR)

Work Package II
Exposure and Toxicology
WP Spokespersons
1. Dr. Hanns-Rudolf Paur (KIT)
2. Prof. Dr. J. Buters (TUM)

Work Package III
Small Molecules and Stable Isotope Labelling
WP Spokespersons
1. Dr. Gunnar Dittmar (MDC)
2. T. Gröger (HMGU)

Work Package IV
Chemometry and Biostatistics
WP Spokespersons
1. N.N.
2. Prof. Dr. O. Wolkenhauer (UR)

Figure 5 | Management structure of HICE.
analytical/biological work packages (WP I-III) in order to link the chemical profile of the aerosol exposure with observed molecular response of the biological system under investigation.

In the actual research, however, the work packages will be highly intercorrelated. Figure 4 shows the iterative workflow for investigation of the effects of a specific aerosol source. The cells are exposed to a well-defined source (WP I) aerosol, gases or particulate of the source and specific biological endpoints are monitored by toxicological tests (WP II). The biological and the composition of the complex aerosol exposure are comprehensively analysed (WP I/WP III). The results of the biostatistical/chemometric data analysis (WP IV) shall allow deeper insight into the early biological effects of aerosol exposure and/or allow the improvement of the conditions for the next exposure experiment.

To foster and intensify the cooperation within HICE, a management structure supervised by a joint scientific steering board was installed, as depicted in Figure 5. HICE is also devoted to the education of graduate students and the promotion of young scientists by means of a joint graduate school program and by establishing a young investigator group. Using internet-based seminars and video transmitted lecture series, the expertise of all national and international partners is available.
HICE Partners
For a description of the overall research activities of the Joint Mass Spectrometry Centre, see the previous section of this report.

The research topic of HICE is well connected to the research program and program-oriented funding of the JMSC at the Helmholtz Zentrum München. Therefore, in addition to the HICE Spokesperson Prof. Dr. Ralf Zimmermann, a large fraction of the JMSC team (staff, graduate students and post graduate students) is involved in the HICE project.

Moreover, the JMSC supports HICE with significant amounts of funding for investments and consumables. HICE is also closely associated with third-party funded projects of the JMSC.

Only the HICE co-workers with the biggest involvement in the HICE research program are expressly listed here. Most of these co-workers are not funded by HICE directly.

**Prof. Dr. Ralf Zimmermann**

Ralf Zimmermann is currently Full Professor and Chair of Analytical Chemistry at the University of Rostock. He is Head of the Joint Mass Spectrometry Centre of the University of Rostock and Helmholtz Zentrum München and Head of the Cooperation Group „Comprehensive Molecular Analytics“ (CMA) at Helmholtz Zentrum München, Neuherberg. He is also Director of the Helmholtz Virtual Institute HICE.

Prof. Zimmermann received his Ph.D. in Physical Chemistry from the Technische Universität München in 1995 and obtained his Habilitation in 2001 at Technische Universität-Weihenstephan. He received a scholarship from the Volkswagen Foundation (1993-1995), the „Fachgruppen“-Award of the Analytical Section of the German Chemical Society in 1999 and the J.B. Phillips Award for Comprehensive Gas Chromatography in 2008. He is the founder of Photonion GmbH (2009).

Ralf Zimmermann has authored more than 170 peer reviewed publications, has earned more than 15 patents, and has delivered more than 370 lectures.
at national/international conferences or during invited institute seminars. His research interests include:

- Mass Spectrometry: Instrument development and applications;
- Photo ionisation mass spectrometry;
- Analysis of complex molecular systems: Food, Tobacco, Crude oil and etc.;
- Industrial process analysis, Petrochemical processes, BTL and CTL technologies;
- Multidimensional comprehensive chromatographic separation techniques;
- Metabolomics, Breath gas analysis;
- High resolution mass spectrometry;
- Environmental analysis;
- Coupling technology, Thermal analysis;
- Aerosol research (Ambient aerosol, Emissions, SOA and etc.);
- Health effects of air pollution and aerosols (Environmental Health);
- Aerosol instrumentation.

Thomas Gröger

Thomas Gröger is a Senior Scientist within the cooperation group CMA at Helmholtz Zentrum München. His work involves the characterisation of complex molecular systems by mass spectrometric techniques, with a special focus on the conceptional research, further development and application of higher dimensional separation techniques.

Erwin Karg

Erwin Karg is also a Senior Scientist within the cooperation group CMA at Helmholtz Zentrum München. His research is focused on the characterisation of particulate and gaseous atmospheric components, the characterisation of particle surface area, experimental aerosol production, instrumentation and analysis and the impact of particulates on human health.

Sophie Klingbeil

Sophie Klingbeil is a Software Engineer from the University of Rostock. Her research covers the preparation and adaptation of Matlab-based routines for automatic data treatment and data analysis.
Jürgen Orasche

Jürgen Orasche is a PhD Student at Helmholtz Zentrum München/University of Göttingen. He is responsible for offline-sampling (particles and gaseous phase), online gas-phase measurements via Fourier-Transform Infrared Spectrometer (FTIR) and online particle size distribution measurements via Electrostatic Low Pressure Impactor (ELPI). Among other analytical approaches, the samples will be characterised via In-situ Derivatization Thermal Desorption Gas Chromatography Mass Spectrometry (IDTD-GC-TOFMS).

Dr. Johannes Passig

Dr. Johannes Passig is a Senior Scientist at the Institute of Chemistry, Division of Analytical and Technical Chemistry, University of Rostock. His fields of research include light sources for single photon ionization, femtosecond spectroscopy and strong field ionization, and development of mass-spectrometric methods.

Christian Radischat

Christian Radischat is a PhD Student at the Institute of Chemistry, Division of Analytical and Technical Chemistry, University of Rostock. He deals with on-line and real-time analysis of organic combustion products and trace components in the exhaust gases from fuel-powered vehicles and exhaust gases formed during the combustion of wood.

Ahmed Reda

Ahmed Reda is a PhD Student at Helmholtz Zentrum München/University of Rostock. He carries out research on the identification and quantification of reactive (semi) volatile organic compounds ((S)VOCs) in emission aerosol in terms of oxygen content.

Dr. Patrick Richthammer

Patrick Richthammer is a Senior Scientist at Helmholtz Zentrum München. His research is focused on the impact of aerosols on cellular metabolism.

Sorana Scholtes

Sorana Scholtes is project manager of the Helmholtz Virtual Institute HICE at Helmholtz Zentrum München, Neuherberg. She is responsible for planning, organization and communication.
**Dr. Thorsten Streibel**

Dr. Streibel is a Senior Scientist at the Institute of Chemistry, Division of Analytical and Technical Chemistry, University of Rostock. His research deals with improving the comprehension of the formation of organic trace compounds originated from thermal processes, such as pyrolysis and combustion. It also includes the investigation of the thermal behaviour and characterisation of fossil and regenerative fuels.

**Babette Werner**

Babette Werner is a PhD Student at Helmholtz Zentrum München/University of Rostock. The objective of her work is the chemical analysis of the response of biological systems on aerosol exposition.

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**Key Publications**

Hanley L, Zimmermann R; Light and molecular ions: The emergence of vacuum UV single-photon ionization in MS, Feature Article, Analytical Chemistry, 81, 4174 (2009).


Bente M, Sklorz M, Streibel T, Zimmermann R; On-line laser desorption-resonance enhanced multiphoton post-ionization mass spectrometry of individual aerosol particles: Molecular source indicators for particles emitted from diesel and gasoline car emission as well as from soft and hard wood combustion, Analytical Chemistry, 80, 8991 (2008).

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**Web**

www.jmsc.de
www.zimmermann.chemie.uni-rostock.de
www.helmholtz-muenchen.de/cma/index.html
Comprehensive Pneumology Center (CPC) / Institute of Lung Biology and Disease (iLBD), Helmholtz Zentrum München

The CPC/iLBD is a translational research center dedicated to pulmonary medicine.

It was founded by three partners: the Helmholtz Zentrum München - German Research Center for Environmental Health (HMGU), the Ludwig-Maximilians-Universität (LMU) with the University Hospital, and the Asklepios Hospital München-Gauting in Germany.

Chronic lung diseases are one of the leading causes of death worldwide; the number of people who die in consequence of a lung disease will increase in the future. However, the research of lung diseases is still at its early stages. Therefore, the overall mission of the CPC/iLBD is to perform cutting edge basic and translational research on chronic lung disease, including chronic obstructive pulmonary disease (COPD), lung cancer, asthma, bronchopulmonary dysplasia (BPD) and pulmonary fibrosis.

The significant contribution of CPC/iLBD to HICE is to offer interventional "proof-of-concept" studies by using animal models for chronic lung disease. This also includes the well characterised cigarette smoke-induced mouse model of COPD. This mouse model provides a unique opportunity to analyse the role of individual pathways for combustion aerosol, particle, and gas phase exposures.

Prof. Dr. Oliver Eickelberg

Oliver Eickelberg is Professor of Medicine at the Ludwig-Maximilians-Universität (LMU), Institute of Experimental Pneumology and Chairman of the Comprehensive Pneumology Center.

He has contributed several key studies, which are concerned with the pathogenic role of the TGF-β superfamily in pulmonary arterial hypertension (PAH) and idiopathic lung fibrosis (IPF). His expertise and research interest focuses on lung tissue remodelling, including the interplay of the lung epithelium with the underlying mesenchyme ("epithelial-mesenchymal crosstalk") in chronic lung diseases with distortion of the epithelial-mesenchymal trophic unit (EMTU), particularly interstitial fibrosis and COPD.
Dr. Ali Önder Yildirim

He is the head of the small animal facility (SMAF) that combines the animal models for chronic lung disease at the CPC/iLBD and is deputy director of the iLBD. His focus area is inflammatory lung diseases, in particular cigarette smoke-related COPD. His research group investigates the underlying mechanisms of the development of the disease and tries to identify new therapeutic targets.

Key Publications

**Prof. Dr. Oliver Eickelberg**


**Dr. Ali Önder Yildirim**


Web

www.cpc-munich.org
www.helmholtz-muenchen.de/en/ilbd/about-ilbd/overview/index.html
Institute of Biomathematics and Biometry, Helmholtz Zentrum München

The research group Stochastic Modelling and Statistics is a research unit of the Institute of Biomathematics and Biometry (IBB) of the Helmholtz Zentrum München.

This research unit is concerned with probabilistic and statistical modelling, classical statistics, as well as statistical analysis and exploration of data. The emphasis is on biological and medical applications. The group has expertise in mathematics, statistics, as well as time series nd image analysis. It consists of scientists with a mathematical, statistical and/or engineering background. There are intimate connections with the analysis, numerical, and computational groups in the IBB, to the experimental institutes at the Helmholtz Zentrum München and also to external institutes, in particular those concerned with genetics, molecular biology and microbiology, pathology and imaging.

Key Publications


Dr. Klaus Hahn

Dr. Hahn has a permanent scientist position at the IBB of the Helmholtz Zentrum München. His main scientific contributions are in the fields of nuclear physics, radiation biology/radiation protection, neuroimaging and neuroscience. After studying theoretical physics at the LMU Munich he obtained his doctoral degree at the University of Tübingen. His contributions cover theoretical, mathematical, numerical and statistical investigations and have led to about 75 refereed papers. He is also engaged in the education of young scientists and co-editor of the International Journal of Biomathematics and Biostatistics.
Dr. Hagen Scherb

Dr. Hagen Scherb is Mathematician and Biostatistician at the Institute of Biomathematics and Biometry (IBB), Helmholtz Centre Munich, German Research Center for Environmental Health (HMGU). He has long experience in the field of environmental health risk assessment.

He is especially interested in mathematical and statistical methods for the analysis of ecological data. He is head of ImStatLab (Image Analysis and Statistics consulting Laboratory), a consulting and service unit intended to serve as an interface between HMGU and external scientists and the diverse IBB groups. This group provides assistance for the solution of practical problems, in particular in image analysis and statistics, but also in other fields of mathematics.

The focus of this unit is on developing image analysis, statistics, and general mathematical methods as an integral part in interdisciplinary research, which requires mathematicians and statisticians to become vital and emancipated partners with subject matter scientists and engineers. Emphasis is on data analysis and data mining under the constraints of variability and uncertainty.

Key Publications

Scherb H, Voigt K; Response to W. Kramer: The human sex odds at birth after the atmospheric atomic bomb tests, after Chernobyl, and in the vicinity of nuclear facilities: comment (doi:10.1007/s11356-011-0644-8), Short Research and Discussion, Environmental Science and Pollution Research, 19 (2012).

Sperling K, Neitzel H, Scherb H; Evidence for an increase in trisomy 21 (Down syndrome) in Europe after the Chernobyl reactor accident, Genetic Epidemiology, 36(1), 48–55 (2012).

Fuß R, Ruth B, Schilling R, Scherb H, Munch JC; Pulse emissions of N2O and CO2 from an arable field depending on fertilization and tillage practice, Agriculture, Ecosystems & Environment, 144(1), 61-68 (2011).

Web

www.helmholtz-muenchen.de/en/ibb
Institute of Epidemiology II, Helmholtz Zentrum München

The Institute of Epidemiology II focuses on the assessment of environmental and lifestyle risk factors that jointly affect major chronic diseases such as diabetes, heart disease and mental health.

Research builds on the unique resources of the KORA cohort, the KORA myocardial infarction registry and the KORA aerosol measurement station.

Aging-related phenotypes have been added to the KORA research portfolio within the frame of the Research Consortium KORA-Age.

The institute has published internationally acknowledged contributions to the identification of risk factors for cardiovascular diseases and diabetes where inflammatory responses triggered by particulate matter or by psychic stress had played an important role.

The institute’s contributions are specifically relevant for the population, as modifiable personal risk factors are being researched that could be influenced by the individual or by improving legislation for the protection of public health.

Prof. Dr. Annette Peters

Prof. Dr. Annette Peters is Director of the Institute of Epidemiology II, Helmholtz Zentrum München (since 2010).

2008-2013: Adjunct Associate Professor at the Department of Environmental Health, Harvard School of Public Health, Boston, USA.

2003-Present: Privatdozent Epidemiology Ludwig-Maximilians University, Munich, Germany.

2007-2010: Head of the Research Units "Epidemiology of Air Pollution Health Effects" and "Epidemiology of Chronic Diseases," Institute of Epidemiology, HMGU, Germany.

2001-2007: Head of the Research Unit "Health Effects of Ambient Particles," Institute of Epidemiology, HMGU, Germany.
Dr. Josef Cyrys

Exposure assessment of indoor and outdoor air pollutants: Dr. Cyrys's research interest is, in particular, the development and validation of new measurement methods for an improved physical and chemical characterization of particles to meet epidemiological requirements. He is interested in the source apportionment, the spatial and temporal variability of fine and ultrafine particles, as well as in the relationship between indoor, outdoor and personal exposure to particulate air pollution.

Dr. Cyrys is team leader of the research unit “Exposure Assessment” of the Helmholtz Zentrum München, Institute of Epidemiology II, and senior scientist at the Environment Science Center, University of Augsburg.

Web
www.helmholtz-muenchen.de/en/epi2/
Department of Medical Radiation Physics and Diagnostics, Helmholtz Zentrum München

The research unit Medical Radiation Physics and Diagnostics (AMSD; Director: Prof. Dr. Christoph Hoeschen) at the HMGU especially works on dose reduction strategies in medical imaging.

In terms of evaluating new diagnostic approaches and radiation metabolomics the AMSD developed methodologies (principal investigator: Dr. Wilfried Szymczak) to use Proton Transfer Reaction Mass Spectrometry PTR-MS breath gas investigations on humans, head space analyses on mice and on-vitro cells. Breath provides a non-invasive window to metabolic processes as trace molecular biomarkers in the blood partition from the blood stream via the alveolar pulmonary membrane into the lungs. In vitro cells release volatile biomarkers directly at the air liquid interface into the headspace. The molecular profile of breath or headspace reflects changes in metabolic processes brought about by abnormal physiologies and biochemistries, such as those which occur in disease.

Prof. Dr. Christoph Hoeschen

Dr. Wilfried Szymczak

Key Publications

Brunner C et al.; Discrimination of cancerous and non-cancerous cell lines by headspace-analysis with PTR-MS, Analytical and Bioanalytical Chemistry, 397(6), 2315-2324 (2010).

Greiter M et al.; Differences in Exhaled Gas Profiles between Patients with Type 2 Diabetes and Healthy Controls, Diabetes Technology & Therapeutics, 12(6), 455-462 (2010).


Web

www.helmholtz-muenchen.de/en/amsd
ZAUM - Center for Allergy and Environment

The Center of Allergy and Environment (ZAUM) is a joint center of the Helmholtz Zentrum München and the Technische Universität München.

ZAUM conducts environmental and basic clinical research. The aim is to understand environmental diseases such as allergies, to assess risks and to develop preventive interventions as well as therapies for established diseases.

The focus of the ZAUM is allergen tolerance. Basic immunological mechanisms are looked upon from two points of view. First: What happens when immunological tolerance is broken? Second: How can immunological tolerance be recovered? Immunological tolerance is primarily controlled by "memory"-cells, the T and B-lymphocytes. Based on intervention with these cells we expect improved and long-term effective therapies for allergy patients.

**Priorities**

The translation of our research results into clinical application is our highest priority. Most experiments are performed in humans and with primary human cells or biopsies. A recent success of our investigations on immune memory, specifically the T cell, was recently published in the NEJM (2011 Jul 21;365(3):231-8) and revealed the antagonistic nature of Th2 and Th1/Th17 in the pathogenesis of atopic eczema and psoriasis, respectively. In cooperation with Novartis and the Imperial College London, we initiated a phase II clinical trial to determine whether VAK694 when combined with subcutaneous immunotherapy leads to long-term immune tolerance to allergen in individuals with seasonal allergic rhinitis (NCT01018693). The design of this essay goes back to preliminary work, which was published in Plos Biology in 2007 (Mantel, Plos Biol 2007, 5:12; 2847) and which showed that IL-4 is an effective inhibitor of Treg-induction. By blocking this mechanism, we expect improved therapy effects by the induction of specific allergen tolerance.

**Prof. Dr. Jeroen Buters**

Jeroen Buters leads the group "Environment", which focuses on the environmental cause of allergies. The group "Environment" mainly investigates how environmental and climatic changes modify the allergenicity of air-borne pollen. Another research topic is the influence of environmental pollution on allergies due to waste products of combustion (fine dust and the organic phase connected to them), and the toxic effects of indoor particulate material from schools.

**Research Projects**

The group discovered that pollen have an at least 10-fold biological
variability when releasing allergens. This result is important for patients with allergies, because symptoms depend on the quantity of the allergen. For the comprehensive investigation of this important correlation, a pan-European project was initiated in order to classify the most common released allergens. The aim, in the interest of the patient, is to develop an early warning system (www.HIALINE.com). This project is sponsored by the European Union. The investigation of anthropogenic agents of combustion (i.e. diesel engine exhaust particles) and their influence on the human immune system is a further project, which is of special relevance for our urbanised environment. Combustion products occur mainly outdoors. Indoor particles are important as well because most individuals stay indoors more than 90% of their time. Our observation is that the indoor fine dust contamination is much higher than outdoors, and that indoor particles (PM10) are toxicologically at least if not more active than outdoor air particles. At present, we analyse the toxicologic impact of airborne particles from elementary schools. The risk deriving from these dusts is presently uncertain. Our organism is not defenseless against environmental agents, but metabolises these chemical agents. Ironically, agents can be generated that are sometimes more toxic than the mother agent. The group integrates the role of these metabolising enzymes and therefore allows preventative measures.

**Dr. Sebastian Öder**

Dr. Öder obtained his PhD in 2011 at the Technical University Munich on the subject "toxicity of particulate matter from school indoor air". The systems used for his thesis are well suited for testing the materials generated in HICE. In addition, Dr. Öder will focus on the allergy-related effects of combustion products. Dr. Öder is currently training to become a registered toxicologist (Fachtoxikologe).

### Key Publications

Buters JTM and the HIALINE working group; Release of Bet v 1 from birch pollen from 5 European countries, Results from the HIALINE study, Atmospheric Environment, in press (2012).


### Web

www.zaum-online.de
The Department of Piston Engines and Internal Combustion Engines was filled with the current Chair Prof. Dr.-Ing. Horst Harndorf in 2006.

The goal was to focus research attention more closely on more traditional strengths of the department, such as research on the use of alternative fuels in internal combustion engines, laser optical injection spray analysis and the analysis of emission-reducing measures for large-and marine diesel engines and to combine these with the current work on developing combustion processes, exhaust after treatment and development of thermodynamically based control algorithms for future engine.

The research activities of the Department are focused on the optimization of energy processes in internal combustion engines and exhaust after-treatment as well as the adaptation of engines to alternative gaseous and liquid fuels. The following major research areas are dealt with:

Analysis of combustion processes in gasoline and diesel engines to gain a better understanding of combustion processes, heat transfer and charge air motion processes in internal combustion engines.


Studies of the injection characteristics of standard and alternative fuels, analysis of jet breakup, the beam propagation and the air inlet of the jet, derivation of optimization concepts.

**Prof. Dr. Horst Harndorf**

Prof. Harndorf holds the chair of Combustion Engines. He has more than 25 years experience in R&D in this area, automotive operation and application of alternative sustainable fuels (natural gas, bio gas, dimethylether, bio fuels and etc.).

~15 years in industry with Robert-Bosch GmbH in a management position before he was appointed professor at the University of Rostock. Beside his lectures at the University of Rostock, he leads several research projects covering exhaust treatment, fuel-mixture generation, heat transfer, tribological problems and application of alternative sustainable fuels.
Dr. Ulrike Schümann

Head of the laboratory for fuels and Lubricants. She supervises several projects concerning influences of alternative sustainable fuels on lubricating oil as well as the influence of fuel blends on the operating behaviour of modern diesel engines. Furthermore she deals with fuel characteristics under extreme conditions. Besides her work at the University of Rostock she is active in several specification organisations and biofuel networks.

Dr.-Ing. Christian Fink

Head of the work group for injection systems and fuel-mixture generation. He studies the impact of common rail injection systems on engine emissions and fuel consumption for several fuels (e.g. diesel blends, heavy fuel oil). Therefore, jet spreading and nebulisation is analysed in a high pressure-high temperature injection chamber and at an engine test-bed by optical and laser optical methods.

Dipl.-Ing. Benjamin Stengel

Research assistant at the Chair of Piston Machines and Combustion Engines. He coordinates and organises HICE-related engine measurement campaigns involving different combustion processes and fuels at the University of Rostock. Moreover, he deals with exhaust sampling and measurement methods in order to achieve comparable results.

Key Publications


Schümann U et al.; Bestimmung des Pflanzenölanteils ingebrauchten Dieselmotorenölen – Motorische Auswirkungen und verfügbare Analysenverfahren, Tribologie und Schmierungstechnik, Heft 04 - 2010, Expert Verlag, Juli-August (2010).


Web

www.lkv.uni-rostock.de/en
HICE NATIONAL PARTNERS

Department of Systems Biology and Bioinformatics, University of Rostock

The Department of Systems Biology and Bioinformatics of the University of Rostock focuses on the development of systems and control methodologies using mathematical modelling and statistical data analysis applied to complex dynamical systems.

We build realistic and useful models of biological phenomena from the molecular level, to cellular, tissue and organismal levels through close collaborations with experimental biologists. Our contribution to HICE is the expertise in mathematical modelling and the description of complex molecular systems. This includes the development of bioinformatics tools and statistical data analysis.

Prof. Dr. Olaf Wolkenhauer

His research interest is in data analysis and mathematical modelling directed towards an understanding of cell function. He received his first degrees in control engineering in 1994 and obtained his PhD from the University of Manchester in 1997 for research on the application of possibility theory to data analysis.

Following a research lectureship at the Control Systems Centre at Manchester and a research fellowship at the Technical University Delft in the Netherlands, he moved to the University of Rostock in Germany in 2003. There he holds the Chair in Systems Biology and Bioinformatics. Since 2005, he has been a fellow of the Stellenbosch Institute for Advanced Study (STIAS) and an Adjunct Professor at Case Western Reserve University, Cleveland, USA.

Key Publications


Web

www.sbi.uni-rostock.de/home
Finite size, large surface fraction, limited capacity for heat and charge, and discrete electron states: These are the characteristics of metal clusters and nanoparticles, addressed in the field of cluster physics.

Clusters and Nanostructures at the Institute of Physics, Rostock University

Prof. Dr. Karl-Heinz Meiwes-Broer
PD Dr. Josef Tiggesbäumker
Dr. Viola von Oeynhausen
Dr. Ingo Barke
Dr. Steffen Fiedler

Our research is aimed at the remarkable consequences, many of which are accessible by spectroscopic means. Free clusters in a beam allow for the investigation of the pure cluster properties where the coupling to the environment may be neglected. When deposited onto a surface the cluster-substrate interaction becomes crucial and is a topic of intense research. The experimental methods comprise a manifold of mass spectroscopic techniques, in order to analyze cluster sizes, to mass-select clusters and nanoparticles in a beam, or as detection tool in linear as well as non-linear laser spectroscopy. Besides different ns laser systems the group uses femtosecond lasers, including pulse shaping and colored double pulse techniques. For high photon energies the free electron laser FLASH in Hamburg can be employed. A large part of the research is conducted within the Sonder-forschungsbereich SFB 652, different BMBF projects, and as part of + the excellence programs "Light to Hydrogen" and "REMEDIS". Within HICE the group will be involved in the development of photoionisation techniques. This includes the implementation of supersonic nozzle beams together with novel light sources. We may note that our HICE work fits well into the activities of the Department Life, Light and Matter at the Rostock University. The department aims at interdisciplinary research and training in the fields photon sciences, engineering and catalysis, regenerative medicine and numerical simulations. The program comprises science within several faculties and institutes of the Rostock University.

Selected Topics of the Group Clusters and Nanostructures

Spectroscopy on Metal Clusters Embedded in Helium Droplets

Ultracold helium nanodroplets provide an interesting superfluid matrix for studies on embedded clusters. The technique of atom pick-up in helium droplets provides a flexible tool to nearly independently adjust the size of both the droplets and the embedded species. For spectroscopy studies, resonant resonant two photon ionisation is applied to mass-select the embedded neutral metal clusters. In combination with photoelectron spectroscopy, the intermediate state
dynamics is to be analyzed. Moreover, exotic species like molecular chains or foam-like structures can be generated. In femtosecond pump-probe studies the formation dynamics of metal ion helium snowballs provides information about the local atomic environment.

**Strong Field Excitations of Molecules and Clusters in the Optical Regime**

Intense femtosecond laser pulses are used to investigate strong-field induced phenomena in small particles. Clusters serve as model systems to interrogate double pulses are much more effective in the generation of these energetic species than ultrashort single pulses. Due to the resonant interaction of the oscillating laser field with the collective mode of cluster electrons, an effective acceleration of electrons can be achieved. Recently we could show that adapted light fields (temporally shaped in amplitude and phase) allow the adjustment of the ionic charge state distribution from strong-field cluster interactions nearly at will.

**Clusters Excited by XUV-light from Free Electron Lasers (FEL)**

The rapid advances in the FEL technology have opened new avenues to drive, control, and analyse the structure and dynamics of matter. Several novel approaches, such as single-shot coherent diffractive imaging or ultrafast time-resolved holography of nanostructures, small particles, or biological samples are presently in reach or have been demonstrated. A crucial fundamental...
question being closely related to all existing and upcoming applications of intense FEL light is how the interaction mechanism of intense laser fields with matter develops in the spectral range from the extreme ultraviolet (XUV) up to the x-ray domain. Atomic clusters are an ideal testing ground for corresponding fundamental studies as great experience in their experimental and theoretical analysis is available. The group is involved in several experiments at FLASH in Hamburg.

**Clusters and Atomic Chains at Surfaces**
The properties of nanoclusters typically change substantially compared to the gas phase when brought into contact with surfaces. In view of potential applications a holistic understanding of the cluster-surface system is inevitable. Our group has experience in generating clusters and nanoparticles with physical methods (sputtering, gas aggregation, laser vaporization, arc discharge, helium pickup). After beam formation, the systems can be mass-selected and deposited onto surfaces. Topics of interest are, e.g., nanomagnetism, or the role of clusters as catalysts. Special interest is in atomic chains, i.e. one-dimensional quantum systems at surfaces. The strongly anisotropic Au-induced reconstruction on silicon can be viewed as the ultimate nanowire. We use those to investigate the physics of electrons in one dimension by scanning tunneling spectroscopy. The results open new routes for quantitative and local control of electron states in metallic nanostructures on the atomic scale.

**Key Publications**

Polei S, Barke I, Erwin S, Meiwes-Broer KH; Periodic variations in the local surface potential of Si(111)- (5x2)-Au, Physical Review B, 85, 165414 (2012).


**Web**
web.physik.uni-rostock.de/cluster/
Karlsruhe Institute of Technology

Karlsruhe Institute of Technology (KIT) is a higher education and research institution with about 8900 employees, 21000 students and an annual budget of 750 million Euros.

KIT was established on October 1, 2009, as a merger of the University of Karlsruhe (founded in 1825), one of Germany’s leading research universities, and Forschungszentrum Karlsruhe (founded in 1956), one of the largest research centres of the Helmholtz Association.

Higher education, research and innovation are the three pillars of KIT’s activities. KIT’s research profile is characterised by a strong focus on energy technology, nanotechnology and materials research, elementary particle and astroparticle physics as well as climate and environmental research. It has significant competencies in the fields of information and communication technologies, mobility systems, optics and photonics, and the inter-relations of humans and technology.

KIT will be involved in HICE with its Institute for Technical Chemistry (ITC) and its Institute for Toxicology and Genetics (ITG).

Institute for Technical Chemistry

The activities of ITC (Head: Prof. Dr.-Ing. H. Seifert) are focused on the development of eco-efficient thermal process technologies for the utilisation of biomass, refuse-derived fuels and alternative fuels in high temperature processes. Technologies like combustion, pyrolysis and gasification and reduction technologies for gaseous and particle-based pollutions will be employed. The processes will be applied to power plants, the chemical industry and basic materials industry and the production of transport fuels (bioliq® process). The experimental research activities comprise basic lab scale investigations, applied research at semi-industrial scale and industrial scale facilities. Model based work complements the research activities.

Dr. Hanns-Rudolf Paur

In the Department Aerosol and Particle Technology (Head: Dr. H.-R. Paur) the whole life cycle of airborne particles is being studied. Objectives include:

To form nanoparticles in high-temperature processes and microwave plasma is measured by a novel particle mass spectrometer. Model calculations are developed and validated by these experimental data.

To remove fine particles from combustion, pyrolysis and gasification novel electrostatic precipitators are developed in fundamental studies. The CAROLA®- Electrostatic Precipitators clean offgas from industrial incinerators and from residential wood combustion.

To quantify and reduce the emission of toxic trace metals from thermal
processes we develop measurement systems and gas cleaning processes. The MercOx®-process cleans the flue gas from hazardous waste incinerators.

To assess the toxicity of nanoparticles and pollutants from biomass combustion processes, the “Karlsruhe Exposure System” (see the image below) was developed. Reproducible amounts of nanoparticles are sampled from emission sources and deposited onto biological interfaces (lung cells, bacteria).

Sonja Mülhopt, Dipl.-Ing. (BA)

Dipl.-Ing. Sonja Mülhopt is responsible for the development of exposure systems for in-vitro studies of nanoparticle toxicology. She has long-term experience in aerosol technologies, including generation and measurement of nanoparticles. She has developed the online dose measurement at the air liquid interface exposure.

Institute for Toxicology and Genetics

Research at the ITG (Head: Prof. Dr. U. Strähle) focuses on the elucidation of molecular and cellular interactions at functional interfaces. A major aim is the identification of molecules that play key roles in cellular signaling, in differentiation and proliferation, during embryonic development, and under pathophysiological conditions. Further topics cover proteomics, genomics and molecular toxicology. Through close cooperation with chemists and physicists, these new findings will be used to guide the rational design of new tools for controlling the behaviour of cells in vivo and in vitro.

Dr. Carsten Weiss

In the research group Molecular Toxicology (Head: PD Dr. Carsten Weiss) different in vitro systems are used to study the toxicity of nanomaterials and particles from combustion processes. These studies are performed under submerged (cells are covered with medium) as well as at the air-liquid interphase (ALI) to simulate

Figure 1 | Compact Karlsruhe Exposure System used to assess the toxicity of nanoparticles and pollutants from biomass combustion. Image source: KIT.
the processes during inhalation of nanomaterials and combustion aerosols. KIT-ITC contributes to WP I by generation and characterisation of test combustion aerosols (from wood combustion) as well as characterisation of combustion aerosols during experimental campaigns. The aerosols are characterised by size distributions and number and mass concentration. The aerosols are provided for the exposure of cell and tissue cultures (see WP 2) using a novel and unique mobile system for exposure of cell cultures at the air-liquid interface, which has been developed at ITC together with Vitrocell. KIT-ITC has planned a next generation exposure system adapted to the requirements of HICE which will be built by ITC in cooperation with Vitrocell supplying especially designed exposure chambers. This HICE exposure system will be used during the experimental campaigns at different sites and emissions sources. Human and animal lung cell cultures as well as a differentiated multi cell-type human lung tissue model from UCA are facilitated and supervised by KIT-ITG. The biological effects of the respective exposures are monitored by toxicological tests. The examined biological endpoints are cytotoxicity, metabolic activity, cellular functions (e.g. metabolism of foreign substances), oxidative stress and inflammatory response markers. The exposed test cells are also processed for further analyses in WP III (proteome, metabolome). Data are evaluated in cooperation with WP IV.

Dr. Silvia Diabaté

Dr. Silvia Diabaté is biologist and has extended experience in the toxicology of combustion-derived particles and nanoparticles, including inflammatory and anti-oxidative processes in lung cells. Together with ITC, she developed the in-vitro assay for investigating the potential toxicity of aerosols after exposure at the air-liquid interface of cells.

Web
www.itg.kit.edu/223.php

Marco Dilger

After finishing his diploma in food chemistry, he started as a joint PhD student of KIT-ITG and KIT-ITC in March 2012. The goal of his PhD thesis is the in vitro characterization of adverse health effects of anthropogenic aerosols. His main tasks in HICE will be a) exposure of test cell cultures at the air-liquid interface, and b) investigation of the toxicological endpoints thereof.

Key Publications


Fritsch-Decker S, Both T, Mülhopt S, Paur HR, Weiss C, Diabaté S; Regulation of the arachidonic acid mobilization in macrophages by combustion-derived particles, Particle and Fibre Toxicology 8(23) (2011).
Max Delbrück Center for Molecular Medicine, Berlin-Buch

The Max Delbrück Center (MDC) for Molecular Medicine is a major biomedical research institute located in the northeastern corner of Berlin, Germany.

The MDC was founded in 1992 with the mission of translating discoveries from molecular research into applications to improve the prevention, diagnosis, and treatment of major human diseases. Translational research, bringing the latest science from the bench to the bedside, is carried out within the framework of the Experimental and Clinical Research Center (ECRC) – the centerpiece of our collaborations with the Charité-Universitätsmedizin. The ECRC combines research labs and several outpatient clinics, clinical training programs, and offers funding for groups and specific translational projects, enabling close collaboration between MDC researchers and clinical scientists of the Charité.

The MDC has placed a special emphasis on systems biology, and a major unit called the Berlin Institute for Medical Systems Biology (BIMSB) has been established to pursue this topic in close collaboration with existing groups. The scientific focus of BIMSB is post-transcriptional gene regulation with a particular emphasis on the role of microRNAs in health and disease.

Work at the institute is supported by high-throughput technology platforms for mass spectrometry, flow cytometry, confocal and two-photon microscopy, electron microscopy and magnetic resonance tomography, along with bioinformatics services and advanced data modeling, for example mathematical cell physiology.

With over 300 PhD students in several graduate programs, the MDC is helping to educate a new generation of scientists. The MDC as a collaborating partner in the HICE consortium will contribute its expertise in large scale proteomics. This will fill the gap between transcriptional regulation and the metabolomic and aerosole analysis data.

Dr. Gunnar Dittmar

Dr. Dittmar leads the group for mass spectrometry based proteomics at Max-Delbrück Center for Molecular Medicine. As the central hub for mass spectrometry the Dittmar group interacts with most of the research groups of the MDC and provides proteomic analysis. The spectrum of proteomic techniques includes quantitative shot-gun as well as targeted proteomics. The shot-gun technology combined with the SILAC technology (stable isotope labeling in cell culture) allows the identification and quantification of several thousand proteins in one experiment. This is the basis of proteomic analysis and comparison of different cell populations. Additionally this technique allows the identification of post-translational modifications, which can act as molecular switches to change the function of proteins in a cellular context.
The mapping of post-translational modifications on the transcriptional activator C/EBP is an example of such a collaboration project which lead to the surprising identification of more than 70 modifications present on this regulatory molecule (Leutz et al., 2011). Contrary to the shot-gun approach targeted proteomics focuses on a limited number of proteins. This concentration on less comes with a gain in sensitivity. This allows to detect proteins in very low concentrations. In a collaboration with the Scheidereit and the Wolf group targeted mass spectrometry was applied to the NFκB system.

Protein Degradation

Protein synthesis and degradation are important for the cellular homeostasis and regulatory events. The cell has several mechanisms to selectively degrade proteins, which are tightly controlled. One of these cellular degradation systems is the ubiquitin-proteasome system. The small protein ubiquitin acts as a degradation signal which is covalently attached to the target protein by an enzymatic cascade. Understanding the impact of ubiquitin-mediated degradation on proteomic level is one of the goals of the Dittmar lab.

Tamara Kanashova

She studied biotechnology at the Otto von Guericke University in Magdeburg (Germany). She finished her studies with a diploma thesis, which she prepared in collaboration with a biotechnology company (AnaTox GmbH & Co KG) on quality control procedures for a dissolution sampler. At the end of January she joined the Dittmar group to work on the characterization of proteomic changes in a aerosol exposed cells.

Key Publications


Web

mdc.helmholtz.de/de/research/core_facilities/cf_mass_spectrometry/teammember/10823_gunnar_dittmar/index.html
The Leibniz Institute for Baltic Sea Research, Warnemünde

The Leibniz Institute for Baltic Sea Research is an independent research institution specializing in the interdisciplinary study of coastal oceans and marginal seas.

The Leibniz Institute for Baltic Sea Research (Leibniz-Institut für Ostseeforschung Warnemünde, IOW) was founded in 1992 on the recommendation of the German Council of Science and Humanities. The IOW is a member of the Leibniz Association (Leibniz-Gemeinschaft, WGL). Its research program focuses on coastal oceans and marginal seas with a particular emphasis on the ecosystem of the Baltic Sea.

The marine chemistry section is concerned with questions of basic research and contributes to the environmental monitoring program of the Baltic Sea. Priorities include the examination of spatio-temporal variations, transport and transformation of chemical variables in marine ecological systems, particularly those of the Baltic. The primary focus of this research is natural and anthropogenic water components, such as gases, nutrients, inorganic carbon compounds, as well as oil components and halogeneous-organic contaminants. The areas of investigation are the water column, suspended particulate matter and sediments, as well as the biota and atmosphere. The Organic Contaminants group investigates the behaviour of organic substances in the marine environment. We study primarily persistent compounds such as polychlorinated biphenyls (PCBs), various pesticides, polycyclic aromatic hydrocarbons (PAHs) and anthropogenic and natural produced volatile halogenated substances, like bromoform.

Prof. Dr. Detlef Schulz-Bull

Prof. Detlef Schulz-Bull is Head of the Marine Chemistry Department, Head of the Analytical Group and Deputy director of IOW.

Key Publications


Web

www.io-warnemuende.de/detlef-schulz-bull-en.html
The University of Luxembourg, founded in 2003, is one of the youngest universities in Europe. It is a research-focused university with about 5000 international students.

Systems biomedicine has been identified as a high priority research area. For this purpose, the government of Luxembourg has launched a major program in personalised medicine, which includes the establishment of a Centre for Systems Biomedicine (LCSB). Rudi Balling was recruited as the founding director of this new Centre in 2009. Within the University of Luxembourg, the Luxembourg Centre for Systems Biomedicine (LCSB) is one of two Interdisciplinary Centres. The focus of the LCSB is on understanding the molecular and cellular mechanisms underlying the development and progression of neurodegenerative diseases through experimental and systems biology approaches. Mathematical descriptions of disease relevant networks are developed and used for the modeling and simulation of how diseases develop and how diseases are influenced by genetic predisposition or by external environmental parameters, such as toxic compounds, drugs, nutrition or life style.

Scientists at the LCSB have intensive knowhow in studying complex biological systems, particularly in disease network inference and analysis. The staff consists of a highly interdisciplinary team of biologists, MD’s, theoretical physicists, computer scientists and engineers trained in systems control and artificial intelligence.

**Metabolomics Platform**

Currently, we routinely analyse intra- and extracellular metabolites in mammalian cells in culture (~100,000 cells), tissue (10 mg) or body fluids like plasma, CSF or urine (5 μl). We developed experimental protocols to
efficiently extract small-molecules from the samples and to prepare them for mass-spectrometric measurement. To analyse the recorded complex raw data, we develop required algorithms and implement those in software tools. Until now, the metabolomics group has developed and applied the software MetaboliteDetector and an R based statistical analysis pipeline.

**Dr. Karsten Hiller**

For a more detailed understanding of cellular metabolism, we develop and apply tools based on stable-isotope tracers. Our group established a technology to determine the metabolic fate of a stable-isotope labeled metabolic precursor: The Non-targeted Tracer Fate Detection (NTFD) system detects all compounds downstream of the tracer without any a priori knowledge.

Our contributions to the research objectives of HICE are:

Discovery: Our stable-isotope assisted and non-targeted technologies allow for the identification of unknown metabolic mechanism induced by exposure to aerosols. Validation: Using stable isotopic metabolic precursors we can determine what biochemical reactions are active in a biological system, by verifying the occurrence of stable-isotopes in metabolites downstream of the precursor. Metabolic flux analysis allows for the determination of quantitative data on enzyme activities. This information are required for parameterising and curating systems-level models describing cellular effects induced by aerosols. Biomarker discovery: Our non-targeted metabolomics measurements provide complex data helping to generate hypothesis and to discover metabolic biomarkers specific for aerosol induced effects.

**Key Publications**


**Web**

www.de.uni.lu/lcsb
The University of Eastern Finland is a multidisciplinary university that is internationally recognised for its competitive research and education.

The university has four faculties: the Philosophical Faculty, the Faculty of Science and Forestry, the Faculty of Health Sciences, and the Faculty of Social Sciences and Business Studies. With approximately 14000 students and 3000 staff members, it is one of the largest universities in Finland.

Inhalation Toxicology Laboratory, Department of Environmental Sciences, Kuopio, Finland

Thematically, research of the inhalation toxicology laboratory is concentrated on the three leading environmental health problems in the developed world:

- Outdoor fine particle air pollution
- Microbial exposures in water damaged buildings
- Increased incidence of asthma and allergies

The overall aim is to identify the actual causes of adverse health effects associated with these indoor and/or outdoor air pollutants by using cell lines, primary cells (e.g clinical samples), and experimental animals. Research in the Inhalation Toxicology Laboratory is carried out focusing on the activation of immunotoxicological mechanisms of adverse health effects induced by source specific combustion emissions.

Protective Role of Environmental Microbes

Beneficial effects of environmental microbial exposure on the maturation of immune responses and development of asthma and allergies in early life.

The open questions concerning causality between exposure and related health impacts can only be addressed in a multidisciplinary experimental environment which makes possible the analysis of the whole chain from emission source via dilution and transformation to health-related toxicological responses in cells and animals. In order to respond to these challenges, the laboratory has close multidisciplinary collaborations with experts in exposure assessment, combustion technology, environmental technology, aerosol physics and epidemiology. Toxicological research is carried out using particles from various combustion processes, engine emissions and nanoparticles.

Research covers studies on proposed toxic mechanisms behind PM-induced adverse health effects including cytotoxicity, inflammation, oxidative stress and genotoxicity. The laboratory has excellent facilities for toxicological studies, including secondary and primary cell culture laboratories, an exposure and analysis laboratory with latest analysing techniques, a cell culture laboratory for air liquid interface, and a controlled weighing room for...
mechanisms of cell death and activation of immunological defense mechanisms of adverse health effects by microbes in indoor air, urban air particulate matter and source specific emissions. The group also participates in studies on microbial exposure and development of allergy and immunological function in early life. She has 154 original peer-reviewed articles in international scientific journals.

Dr. Pasi Jalava

Dr. Jalava graduated in 2003 from M.Sci program of Applied Zoology at the University of Kuopio. He did his Ph.D in Environmental Health for University of Kuopio and graduated in 2008. During Ph.D studies he was working in National Public Health Institute of Finland. Pasi Jalava has about 9 years experience in toxicological studies of air pollution particles. He has a strong background in different studies of air pollution, e.g. research on inflammation, cytotoxicity, genotoxicity and oxidative stress, induced by particulate matter from outdoor air, combustion sources and diesel engines. Since 2005, he has published 19 original peer reviewed articles in appreciated international journals and presented his findings in several international conferences. He has worked on several national and international research projects that have been funded by European Union Framework programmes, Tekes, and European regional development and social funds. He has also worked in Kantiva bioenergy research center of University of Eastern Finland where he has been coordinating of advancement of the toxicological research related to bioenergy production and use. He is supervisor in three current PhD thesis projects at UEF. Pasi Jalava will start his post doctoral period of one year in Fraunhofer

Prof. Dr. Maija-Riitta Hirvonen

Prof. Hirvonen graduated in 1986 from the M.Sci program (Environmental sciences) at the University of Kuopio (now University of Eastern Finland, UEF) and in 1991 with a PhD degree in toxicology at the same university. For post doctoral studies, from 1992 to 1994, she joined Burroughs Wellcome Co., Department of Cell Biology, USA.

Since 1994 she has been docent in environmental toxicology at the faculty of Natural and Environmental Sciences, University of Kuopio. In 2007 she was appointed as research professor at the Public Health Institute (now National Institute for Health and Welfare, THL) and professor in environmental toxicology at UEF. Since January 1, 2011, she has been Vice-Dean in the Faculty of Natural Sciences and Forestry at UEF.

She is the leader of the toxicology group on air pollution in vitro and in vivo. The multidisciplinary studies of her research group are focused on
Institute for Toxicology and Experimental Medicine starting from May 2012. Jalava is working in novel multidisciplinary research line for aerosol toxicology at UEF. The air-liquid-interface systems, developed will form basis for the high quality research in the aerosol toxicology.

**Key Publications**


**Web**

www.uef.fi/intola

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**Fine Particle and Aerosol Technology Laboratory (FINE), Department of Environmental Sciences, Kuopio, Finland**

Research carried out in the Fine Particle and Aerosol Technology Laboratory is focused on aerosols and high temperature processes. The main research areas and strengths are fine and nanoparticles in material synthesis and combustion. Research is carried out on fine particle issues in various combustion processes, engine emissions, nanoparticle synthesis and health&safety aspects as well as aerosol sampling, dilution and characterisation techniques. The research area covers the complete chain from fine and nanoparticle particle formation and behaviour all the way up to the sampling and dilution of particles into the ambient air and their health risks. In material synthesis the main focus is on gas phase synthesis of nanoparticles with atmospheric pressure chemical vapour deposition (APCVD) and physical vapour deposition (PVD) methods. In the FINE laboratory, the staff includes 21 members: a professor, 4 post docs and 12 doctoral students, a secretary, a service engineer and 2 graduate students.

**Prof. Dr. Jorma Jokiniemi**

Prof. Jokiniemi received his Ph.D. in 1990 from the University of Helsinki on the topic „The effect of airborne hygroscopic matter on aerosol behaviour in severe nuclear power plant accidents” after graduating from the University of Helsinki in 1984. In 1991 his research interest moved to combustion aerosols and chemistry. In 1995 he received the status of docent from Helsinki University of Technology. In 2005 he was appointed as professor of fine particle technology.
at the University of Kuopio and research professor on the same topic at Technical Research Centre of Finland (VTT). From 1991 to 2005 he was the head of the research group „Aerosol Technology“ at VTT, and since 2005 he has been the Director of the „Fine Particle and Aerosol Technology Laboratory – FINE“ at the University of Eastern Finland. Prof. Jokiniemi has over 28 years experience in fine particle and aerosol research. He has supervised eight doctoral theses, 109 peer-refereed papers, more than 500 other publications and nine patents.

Key Publications


Olli Sippula, Ph.D.

Olli Sippula received a Master’s degree on Environmental Engineering at the University of Oulu in 2004 and a PhD degree on Environmental Science at the University of Eastern Finland in 2010. He has nine years of experience in studies related to combustion aerosols, emission reduction technologies, fine particle sampling methods and ash behaviour and chemistry in biomass combustion. He has worked as a development manager in the Kantiva bioenergy research center of UEF and as project manager in a number of research projects. He is currently a supervisor of four Ph.D. theses and has about 70 publications of which 14 are original peer reviewed articles. He started a one year post-doctoral period at the University of Rostock in the Joint Mass Spectrometry Centre in June 2012.

Key Publications


Web
www.uef.fi/fine
The Cardiff School of Biosciences is best known for the work of its former director, Professor Sir Martin Evens Frs. This work was recognized by Sir Martin's Nobel Prize in Physiology or Medicine 2007 (together with Mario Cappechi and Oliver Smithies) "for their discoveries of principles for introducing specific gene modifications in mice by the use of embryonic stem cells". Under its current director, Medical Research Council Professor Ole Petersen CBE FRS, who pioneered patch clamp single channel recordings in epithelial cells and discovered intracellular calcium tunnels in exocrine gland cells, the School provides a dynamic and stimulating research environment with impressive modern facilities and high-calibre research-active staff. The Cardiff School of Biosciences is one of the largest bioscience departments in the UK. Supported by state-of-the-art facilities, its topical courses and cutting-edge research spans the full range of the Life Sciences from whole (eco) systems to molecular biology.

**Dr. Kelly BéruBé**

She is the Director of the Lung & Particle Research Group at the School of Biosciences, Cardiff University, UK. With a background in electron microscopy and lung toxicology, she has built an international reputation in the field air pollution and human health and holds numerous appointments in the USA and UK on funding bodies, advisory councils, professional societies and journal editorial boards that focus on environmental health. Her research focuses on the determination of intelligent biomarkers of exposure and harm in the respiratory system, with a particular interest in understanding how pollutants compromise lung biochemistry and alter gene and protein expression to drive disease mechanisms.

Dr. BéruBé's research has been recognised with a number of awards, including the Institute for Science & Health (USA) "Scientific Merit Award 2006" for toxicogenomics of inhaled xenobiotics and the honour of being the British Toxicology Society "Australasia Visitor 2006" to conduct a coast-to-coast lecture tour on nano-toxicology. Current work on "human tissue equivalents of respiratory epithelia", as viable in vitro alternatives for in vivo inhalation toxicology, was awarded the UK NC3Rs "Replacement Prize" and the "Science & Technology Innovation Prizes" in 2007 and 2010. Dr BéruBé's field of study is of natural interest to the general public, and as such, she is a prolific science writer and popular invited speaker, and has worked extensively on communicating her research through public engagements of science for primary schools, laymen groups and professional learned societies.

**Dr. Tim Jones**

- Director of Taught Postgraduate Programmes;
- Head of Applied Environmental Geoscience Research Group;
Joint leader of the Particle and Lung Research Group;

- Deputy directory, M.Sc. Applied Environmental Geology;
- Admissions Officer MSc.

Dr. Tim Jones is co-leader of the interdisciplinary Particles and Lung Research Group (PLRG) with Dr. Kelly BéruBé in Biosciences, Cardiff. The PLRG won the IFSH Dietrich Hoffman Scientific Merit Award in 2006, and the NC3Rs Replacement prize 2007.

**Ailsa Langford**

Is a recent graduate from the School of Biosciences, Cardiff University, Wales, UK. She graduated with a BSc (1st class, honours) degree in Biomedical Science. Her PhD project will involve the „determination of the oxidative capacity of air pollution from different European Union pollution zones“. This project will be supervised by Dr. Kelly BeruBe and Dr. Tim Jones (Cardiff University, UK) and Professor Ralf Zimmerman (Rostock University, DL).

**Image 1 | From left to right:** Tim Jones, Kelly BéruBé and Ailsa Langford.

**Web**
www.cardiff.ac.uk/biosi

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**Key Publications**


Dr T. Jones (PI) and Prof. C. Harris (EARTH), Dr K. BeruBe (BIOSCI).

ASG Analytik-Service Gesellschaft

ASG is an independent, privately owned service provider.

Fields of activity include analytical laboratory for solid, liquid and gaseous fuels, consulting services, process optimisation, production of QC materials and test fuels, and manufacture of instruments for fuel analysis and emissions.

As the first European laboratory with an ISO 17025 accreditation for biofuels, we primarily specialise in answering all analytical and technical questions concerning biodiesel, bioethanol and vegetable oil fuels. Our analytical service comprises testing of all parameters according to national and international specifications (EN 14214, ASTM D 6751, DIN 51605, etc.).

Furthermore, we proudly present our new ASG Customer Center for Biodiesel Process Development. Here you can carry out the whole process chain yourself: From the raw material to the end product with our mini-plant laboratory.

Dr. Thomas Wilharm

Dr. Wilharm is general manager of ASG Analytik-Service Gesellschaft. His professional experience includes:

- Work experience in the field of biofuels since 1993;
- Member of CEN working group 632.1, biodiesel specification;
- Member of CEN TC 307 JWG Validation of EN 14214;
- Quality auditor for the German biodiesel industry and the international BIPAC program of AGQM;
- Member of the European „Bioscopes“ project: Development of biodiesel testing methods;
- Various projects: Process improvement for the biodiesel industry.

Web
www.asg-analytik.de/Firmenprofil_E.html
VITROCELL® Systems GmbH

VITROCELL® Systems GmbH as over 10 years of experience in the development, production, installation, and training for advanced equipment for in vitro studies.

We deliver turnkey systems with a perfect match of all components. Our team consists of competent specialists in research, design and precision manufacturing. Our philosophy is to innovate by working very closely with the customer and to install customised solutions. All equipment is designed using latest state-of-the-art CAD systems in order to allow a realistic judgement of the feasibility prior to the start of manufacturing. The integration of highly qualified workmanship such as boron silicate glass blowing, high-precision engineering components and automation is our strength.

**Contribution to HICE**

Design and delivery of cell culture exposure systems.

**Tobias Krebs**

Tobias Krebs was born in 1956; Managing Partner and Founder; Industrial Engineer, Munich Polytechnic and MBA, INSEAD.

**Figure 1 | VITROCELL® Cultivation and Exposure Systems.** The systems are used for the exposure of aerosols to lung cells at the air/liquid interface. The company produces a broad range of modules for cell culture inserts in 6-well, 12-well and 24-well sizes. The customer receives complete solutions for the smaller lab as well as for higher throughput.

**Web**

[www.vitrocell.com](http://www.vitrocell.com)
Decodon GmbH

Decodon GmbH is a bioinformatics company that develops innovative software for the modern life sciences. Its bioinformatics tools are helping scientists to generate knowledge from the massive amounts of data that are accumulated by recent methods in global functional genomics.

The company brings together specialists with diverse backgrounds from Molecular Biology, Computer Science and Mathematics. Software development at DECODON is driven by the needs of leading researchers in the field of functional genomics and realised by using advanced methods from various areas of Mathematics and Informatics. DECODON's products prove the efficiency of this approach.

The company has its offices in Greifswald, in direct neighborhood to biotech companies as well as the institutes of Micro and Molecular Biology, and Mathematics and Computer Science at the University of Greifswald. Close cooperation with these and other academic institutions gives DECODON access to state of the art technology and methods in both Life Sciences and Informatics. Cooperations exist with companies providing complementary products.

DECODON is a well-positioned niche company with cutting-edge technology, a professional development team and highly qualified management. DECODON is well known in the academic and industrial proteomics markets and wants to further penetrate those markets.

Web
www.decodon.com
Photonion GmbH

Photonion is an innovative company dedicated to providing customised solutions for mentoring chemical compounds.

Photonion GmbH was founded in 2009 as a spin-off from Helmholtz Zentrum München. Wolf Münchmeyer and Dr. Andreas Walte are the founders and general managers of Photonion GmbH.

The goal of Photonion is to develop and distribute new analytical devices based on mass spectrometric methods in order to analyse complex organic gases, liquids or solid materials. Potential applications include process control at combustion, pyrolysis or roasting plants. The analysis of cigarette smoke, of polymers, or crude oil are further applications. Soft ionisation methods, in particular the ionisation with UV light is preferred.

The actual technology is based on one-photon ionisation, based on an innovative vacuum ultraviolet light source. The advantage of this ionisation method is that substances can be measured directly in complex mixtures. Time-consuming separation techniques combined with MS (e.g. GC) are not needed. This is why MS containing soft ionisation is ideally suited for process monitoring and quality control applications.

The headquarters of Photonion are located in Schwerin (Hagenower Str. 73, 19061 Schwerin, Germany) and the research and development division are located in Munich (Helmholtz Zentrum München, building 38c, Ingolstädter Landstr. 1, 85764 Neuherberg, Germany).

Wolf Münchmeyer

Dr. Andreas Walte

Web
www.photonion.de
JRC and Sustainable Transport Unit (STU) – VELA Laboratory

The Joint Research Centre is the scientific and technical arm of the European Commission.

The mission of the JRC is to provide scientific advice and technical know-how to support a wide range of EU policies. Its status as a Commission service, which guarantees independence from private or national interests, is crucial for pursuing its mission.

The JRC has seven scientific institutes, located at five different sites in Belgium, Germany, Italy, the Netherlands and Spain, with a wide range of laboratories and unique research facilities. Through numerous collaborations, access to facilities is granted to scientists from partner organizations.

Many of the complex challenges ahead cut across traditional policy boundaries and require multi-disciplinary research. In order to deliver the best support, the JRC focuses its efforts on seven thematic areas, which respond to major EU and global challenges and take into account the JRC’s proven competences. One of the seven institutes of the JRC is the Institute for Energy and Transport. Inside this structure and since early 2000 the Sustainable Transport Unit (formerly Transport and Air Quality Unit) has been supporting the development and implementation of the future European emissions standards through research strongly based on experimental activities conducted in its Vehicle Emissions Laboratory (VELA). The VELA laboratory is one of the very few laboratories in Europe where all kinds of vehicles can be tested for complete emission characterization.

Several projects supporting key EU emission policies have been carried out and completed in the recent years. A visible example is the validation of the methodology to measure particle number of particles emitted by diesel vehicles and the related emission limit which is now part of the current Euro 5 emission standards.

More recently the attention was focused on the emissions from modern and new vehicle concepts under laboratory and real world driving conditions with conventional and alternative fuels. Moreover, the emission data collected have allowed updating the emission factors of regulated and unregulated pollutants of contemporary engine/vehicle technologies running on conventional and alternative fuels (gaseous fuels and biofuels). This activity is of great important to estimate the contribution of traffic to air pollution which is still a big problem in many European urban areas.

Dr. Maria C. Astorga Llorens

She is senior scientific officer and project leader at JRC-Sustainable transport Unit. She is in charge of the development and implementation of the analytical techniques to characterize...
unregulated pollutants emitted by vehicles. She has followed the application of innovative techniques, like the use of FT-IR instruments to monitor on-line specific compounds in the exhaust emissions. From 2010, she has been co-chairing the United Nations working group in charge of identifying currently unregulated pollutants which will be included in future worldwide harmonized test procedure for light duty vehicles.

Image 1 | VELA experimental facility for Light Duty vehicles and mobile smog chamber from PSI during 2011 campaign in Ispra (Italy).

**Thematic Areas**

- Towards an open and competitive economy;
- Development of a low carbon society;
- Sustainable management of natural resources;
- Safety of food and consumer products;
- Nuclear safety and security;
- Security and crisis management;
- Reference materials and measurements.

**Web**

et.jrc.ec.europa.eu
Acronyms and Abbreviations
# Acronyms and Abbreviations

<table>
<thead>
<tr>
<th>Acronym</th>
<th>Description</th>
</tr>
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<tbody>
<tr>
<td>2D</td>
<td>two-dimensional</td>
</tr>
<tr>
<td>3D</td>
<td>three-dimensional</td>
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<tr>
<td>AAAR</td>
<td>American Association for Aerosol Research</td>
</tr>
<tr>
<td>AAS</td>
<td>atomic absorption spectrometry</td>
</tr>
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<td>ACS</td>
<td>American Chemical Society</td>
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<tr>
<td>AG</td>
<td>working group / corporation</td>
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<td>AMS</td>
<td>aerosol mass spectrometer</td>
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<td>ANOVA</td>
<td>analysis of variance</td>
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<td>APPI</td>
<td>atmospheric pressure photo-ionization</td>
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<td>APS</td>
<td>aerodynamic particle sizer</td>
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<td>ASG</td>
<td>Analytik-Service Gesellschaft mbH</td>
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<td>AUF</td>
<td>Faculty of Agricultural and Environmental Sciences</td>
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<td>BAP</td>
<td>benz[a]pyrene</td>
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<td>BAT</td>
<td>British American Tobacco</td>
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<td>BB</td>
<td>biomass burning</td>
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<td>BBOA</td>
<td>biomass burning organic aerosol</td>
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<td>BC</td>
<td>black carbon</td>
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<td>BESSY</td>
<td>Berliner Elektronenspeicherring-Gesellschaft für Synchrotronstrahlung</td>
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<td>BET</td>
<td>Brunauer, Emment and Teller</td>
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<tr>
<td>bifa</td>
<td>bifa Environmental Institute</td>
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<td>BKA</td>
<td>Federal Criminal Police Office (Bundeskriminalamt)</td>
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<td>BMBF</td>
<td>Federal Ministry of Education and Research</td>
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<td>BMK</td>
<td>Benzomethylketone</td>
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<td>BtL</td>
<td>biomass to liquid</td>
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<td>CE</td>
<td>capillary electrophoresis</td>
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<td>DESCRIPTION</td>
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<td>CHAMP</td>
<td>Collaborative Harmonisation of Methods for Profiling of Amphetamine Type Stimulants</td>
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<td>CI</td>
<td>chemical ionization</td>
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<td>CID</td>
<td>collision induced dissociation</td>
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<td>COD</td>
<td>coefficient of divergence</td>
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<td>CPC/HMGU</td>
<td>Comprehensive Pneumology Center, HMGU</td>
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<td>CSC</td>
<td>Chinese Scholarship Council</td>
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<td>cytochromes P450</td>
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<td>DAAD</td>
<td>German Academic Exchange Service</td>
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<td>DAD</td>
<td>diode-array detector</td>
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<td>DEP</td>
<td>diesel exhaust particles</td>
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<td>DFG</td>
<td>German Research Foundation</td>
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<td>DGMS</td>
<td>German Mass Spectrometry Society (Deutsche Gesellschaft für Massenspektrometrie)</td>
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<td>DGUV</td>
<td>German Social Accident Insurance (Deutsche Gesetzliche Unfallversicherung)</td>
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<td>dehydroabietic acid</td>
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<td>DRI</td>
<td>Desert Research Institute</td>
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<td>DSC</td>
<td>differential scanning calorimetry</td>
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<td>DTD</td>
<td>direct thermal desorption</td>
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<td>DTG</td>
<td>differential thermogravimetry</td>
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<td>DZD</td>
<td>German Diabetes Center</td>
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<td>EAC</td>
<td>European Aerosol Conference</td>
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<td>EBEL</td>
<td>electron-beam pumped rare gas excimer light source</td>
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<td>EC</td>
<td>elemental carbon</td>
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<td>EC-JRC</td>
<td>European Commission Joint Research Institute</td>
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<td>EI</td>
<td>electron impact</td>
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<td>ELPI</td>
<td>electrical low pressure impactor</td>
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<td>EPA</td>
<td>Environmental Protection Agency</td>
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<td>ESI</td>
<td>electrospray ionization</td>
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<td>EU</td>
<td>European Union</td>
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<tr>
<td>Acronym</td>
<td>Definition</td>
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<tr>
<td>FACSS</td>
<td>Federation of Analytical Chemistry and Spectroscopy Societies</td>
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<td>FAME</td>
<td>fatty acid methyl ester</td>
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<tr>
<td>FI</td>
<td>field ionization</td>
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<td>FKZ</td>
<td>grant application number</td>
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<td>FNF</td>
<td>filtered noise field</td>
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<td>FT</td>
<td>Fischer-Tropsch</td>
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<td>FT-ICR-MS</td>
<td>Fourier transform ion cyclotron resonance mass spectrometer</td>
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<tr>
<td>GC</td>
<td>gas chromatography</td>
</tr>
<tr>
<td>GC</td>
<td>two-dimensional „comprehensive“ gas chromatography</td>
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<td>GC-MS</td>
<td>gas chromatography-mass spectrometry</td>
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<td>GDCh</td>
<td>German Chemical Society</td>
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<td>GKS</td>
<td>GKS Gemeinschaftskraftwerk Schweinfurt GmbH</td>
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<td>HBFG</td>
<td>Higher Education Institutions Act</td>
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<tr>
<td>HCA</td>
<td>hierarchical cluster analysis</td>
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<td>Helmholtz-Enterprise-Fonds</td>
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<td>HEL</td>
<td>heating oil</td>
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<td>HGF</td>
<td>Helmholtz Association of German Research Centers</td>
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<td>HMGU</td>
<td>Helmholtz Zentrum München - German Research Center for Environmental Health</td>
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<td>HMTD</td>
<td>Hexamethylene triperoxide diamine</td>
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<td>HOA</td>
<td>hydrocarbon-like organic aerosol</td>
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<td>HPLC</td>
<td>high performance liquid chromatography</td>
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<td>HPLC-MS</td>
<td>high performance liquid chromatography-mass spectrometry</td>
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<td>HRGC</td>
<td>high resolution gas chromatography</td>
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<td>high resolution mass spectrometry</td>
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<td>HR-TOF-AMS</td>
<td>high resolution time of flight aerosol mass spectrometer</td>
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<td>Helmholtz-Zentrum Berlin</td>
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<tr>
<td>I.D.</td>
<td>inner diameter</td>
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<td>ICAS</td>
<td>International Congress on Analytical Sciences</td>
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<td>Acronym</td>
<td>Description</td>
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<td>ICCPA</td>
<td>International Conference on Carbonaceous Particles in the Atmosphere</td>
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<td>ICP</td>
<td>inductively coupled plasma</td>
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<td>IDTD</td>
<td>in situ derivatisation thermal desorption</td>
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<tr>
<td>IDTD-GC-MS</td>
<td>mass desorption gas chromatography mass spectrometry</td>
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<tr>
<td>IDTD-GC-TOFMS</td>
<td>in-situ derivatisation thermal desorption method followed by gas chromatography and time-of-flight mass spectrometry</td>
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<tr>
<td>IEG</td>
<td>Institute of Experimental Genetics</td>
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<td>IEs</td>
<td>ionisation energies</td>
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<td>Institute for Occupational Safety and Health of the German Social Accident Insurance</td>
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<td>Institute of Catalysis Research and Technology, KIT</td>
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<td>Institute of Lung Biology and Disease, HMGU</td>
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<td>Institute for Meteorology and Climate Research - Atmospheric Aerosol Research/KIT</td>
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<td>ion-mobility mass spectrometry</td>
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<td>Faculty of Interdisciplinary Research, University of Rostock</td>
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<td>IÖC</td>
<td>Institute of Ecological Chemistry</td>
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<td>IOW</td>
<td>The Leibnitz Institute for Baltic Sea Research, Warnemünde</td>
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<td>ISCCE</td>
<td>International Symposium on Capillary Chromatography and Electrophoresis</td>
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<td>ISPAC</td>
<td>International Society for Polycyclic Aromatic Compounds</td>
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<td>IPs</td>
<td>ionisation potentials</td>
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<td>IRMS</td>
<td>isotope ratio mass spectrometry</td>
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<td>ITC/KIT</td>
<td>Institute of Technical Chemistry, KIT</td>
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<td>ITG/KIT</td>
<td>Institute of Toxicology and Genetics, KIT</td>
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<td>ITMS</td>
<td>ion trap mass spectrometer</td>
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<td>JMSC</td>
<td>Joint Mass Spectrometry Centre</td>
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<td>JRC</td>
<td>European Commission Joint Research Centre</td>
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<td>K-AMS</td>
<td>potassium aerosol mass spectrometer</td>
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<td>Acronym</td>
<td>Description</td>
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<td>KIT</td>
<td>Karlsruhe Institute of Technology</td>
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<td>KT</td>
<td>Criminal Technical Institute</td>
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<td>LC-MS</td>
<td>liquid chromatography-mass spectrometry</td>
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<tr>
<td>LD</td>
<td>laser desorption</td>
</tr>
<tr>
<td>LDI</td>
<td>laser desorption/ionization</td>
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<tr>
<td>LEZ</td>
<td>Low Emission Zone</td>
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<tr>
<td>LfU</td>
<td>Bavarian Environment Agency</td>
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<td>LIAD</td>
<td>laser-induced acoustic desorption</td>
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<td>LIKAT</td>
<td>Leibniz Institute for Catalysis</td>
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<td>LSD</td>
<td>lysergic acid diethylamide</td>
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<td>LÜB</td>
<td>Bavarian Hygienic Air National Surveillance System</td>
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<td>LWF</td>
<td>Bayerische Landesanstalt für Wald und Forstwirtschaft</td>
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<tr>
<td>m/z</td>
<td>mass-to-charge ratio</td>
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<tr>
<td>MAAP</td>
<td>multi angle absorption photometer</td>
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<tr>
<td>MALDI</td>
<td>matrix-assisted laser desorption/ionization</td>
</tr>
<tr>
<td>MDC</td>
<td>Max Delbrück Center for Molecular Medicine</td>
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<tr>
<td>MDMA</td>
<td>3,4-methylenedioxy-N-methylamphetamine</td>
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<td>MEF</td>
<td>Medical Faculty of the University of Rostock</td>
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<td>MNF</td>
<td>Faculty of Mathematics and Natural Sciences, University of Rostock</td>
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<tr>
<td>MONARPOP</td>
<td>Monitoring Network in the Alpine Region for persistent and other Organic Pollutants</td>
</tr>
<tr>
<td>MOUDI</td>
<td>micro-orifice uniform-deposit impactor</td>
</tr>
<tr>
<td>MS</td>
<td>mass spectrometry</td>
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<tr>
<td>MSTFA</td>
<td>based on silylation with N-Methyl-N-trimethyl-silyltrifluoroacetamide</td>
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<td>MWF</td>
<td>metal working fluid</td>
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<td>Nd:YAG-Laser</td>
<td>neodymium-doped yttrium-aluminum garnet laser</td>
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<td>NIST</td>
<td>National Institute of Standards and Technology</td>
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<td>NMR</td>
<td>nuclear magnetic resonance</td>
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<td>NTD</td>
<td>needle trap device</td>
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<td>NZO-Maus</td>
<td>New Zealand obese mouse</td>
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<td>Acronym</td>
<td>Description</td>
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<tr>
<td>OA TOF-MS</td>
<td>orthogonal acceleration TOF-MS</td>
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<td>OC</td>
<td>organic carbon</td>
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<td>OM</td>
<td>oil mist</td>
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<td>OOA</td>
<td>oxidized organic aerosol</td>
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<td>OPO</td>
<td>optical parametric oscillator</td>
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<td>OWI</td>
<td>Oel-Waerme-Institut GmbH</td>
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<tr>
<td>PAH</td>
<td>polycyclic aromatic hydrocarbon</td>
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<tr>
<td>PAMINA</td>
<td>Particulate Matter in Indoor and Ambient Environments</td>
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<td>PCA</td>
<td>principal component analysis</td>
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<td>PETN</td>
<td>pentaerythritol tetranitrate</td>
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<td>phenanthrene</td>
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<td>PI</td>
<td>photo ionisation</td>
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<td>PI-MS</td>
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<td>PLS-DA</td>
<td>partial least squares discriminant analysis</td>
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<td>PM</td>
<td>particulate matter</td>
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<tr>
<td>PM</td>
<td>particles &lt;=10 µm aerodynamic diameter</td>
</tr>
<tr>
<td>PM2.5</td>
<td>particles &lt;=2.5 µm aerodynamic diameter</td>
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<td>PMF</td>
<td>positive matrix factorisation</td>
</tr>
<tr>
<td>PMT</td>
<td>photomultiplier tube</td>
</tr>
<tr>
<td>PMx</td>
<td>particulate matter with aerodynamic diameter smaller than x µm</td>
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<tr>
<td>POP</td>
<td>persistent organic pollutants</td>
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<td>POPALP</td>
<td>Evaluation of Persistent Organic Pollutants in the Bavarian Alps</td>
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<td>ppb</td>
<td>parts per billion</td>
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<td>ppm</td>
<td>parts per million</td>
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<td>ppt</td>
<td>parts per trillion</td>
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<td>PROT</td>
<td>Research Unit Protein Science, Helmholtz Zentrum München</td>
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<td>PSI</td>
<td>Paul Scherrer Institute</td>
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<td>PTR-MS</td>
<td>proton transfer reaction mass spectrometry</td>
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<tr>
<td>Py</td>
<td>pyrolysis</td>
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<tr>
<td>Acronym</td>
<td>Description</td>
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<td>Py-FIMS</td>
<td>pyrolysis field ionization mass spectrometry</td>
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<td>pyrolysed organic matter</td>
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<td>QIT</td>
<td>quadrupole ion trap</td>
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<td>QMS</td>
<td>quadrupole mass spectrometer</td>
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<tr>
<td>Q-TOF</td>
<td>quadrupol time-of-flight mass spectrometer</td>
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<td>RDI</td>
<td>rotating drum impactor</td>
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<td>RDX</td>
<td>cyclotetramethylenetetranitramine, hexogen</td>
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<td>REMPI</td>
<td>resonance enhanced multi photon ionization</td>
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<td>ROS</td>
<td>Reactive organic species</td>
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<td>RSD</td>
<td>relative standard deviation</td>
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<td>RTE</td>
<td>reactive thermal extraction</td>
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<tr>
<td>SAFE-XUV</td>
<td>Trace Detection of Security Relevant Substances within Complex Matrices</td>
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<td>SD-band</td>
<td>standard deviation band</td>
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<td>SMPS</td>
<td>scanning mobility particle sizer</td>
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<td>SOA</td>
<td>secondary organic aerosol</td>
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<td>SOCAR</td>
<td>State Oil Company of Azerbaijan Republic</td>
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<td>SOFAZ</td>
<td>State Oil Fund of Azerbaijan Republic</td>
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<td>SOM</td>
<td>soil organic matter</td>
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<td>SP</td>
<td>single-particle</td>
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<td>SPE</td>
<td>solid-phase extraction</td>
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<td>SPI</td>
<td>single-photon ionization</td>
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<tr>
<td>SPI-MS</td>
<td>single photon ionisation mass spectrometry</td>
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<td>SPI-TOFMS</td>
<td>photon ionization time-of-flight mass spectrometry</td>
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<td>SPME</td>
<td>solid-phase microextraction</td>
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<td>SRM</td>
<td>standard reference material</td>
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<tr>
<td>SSA</td>
<td>specific surface areas</td>
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<td>SVOC</td>
<td>semi volatile organic compounds</td>
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<td>SWS</td>
<td>weakly teaching hours per semester</td>
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<td>TA</td>
<td>thermal analysis</td>
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<tr>
<td>TD</td>
<td>thermo-desorption</td>
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<tr>
<td><strong>TD-REMPI-SP-TOF-MS</strong></td>
<td>thermo-desorption resonance enhanced multi photon ionization mass spectrometer</td>
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<tr>
<td><strong>TE</strong></td>
<td>thermal extraction/extractor</td>
</tr>
<tr>
<td><strong>TFMPP</strong></td>
<td>trifluoromethylphenylpiperazine</td>
</tr>
<tr>
<td><strong>TFZ</strong></td>
<td>Bavarian Technology and Support Centre</td>
</tr>
<tr>
<td><strong>TG</strong></td>
<td>thermogravimetry</td>
</tr>
<tr>
<td><strong>THM</strong></td>
<td>thermally assisted hydrolysis and methylation</td>
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<tr>
<td><strong>TIC</strong></td>
<td>total ion current</td>
</tr>
<tr>
<td><strong>TMAH</strong></td>
<td>tetramethylammonium hydroxide</td>
</tr>
<tr>
<td><strong>TNT</strong></td>
<td>trinitrotoluol</td>
</tr>
<tr>
<td><strong>TOFMS</strong></td>
<td>time-of-flight mass spectrometry</td>
</tr>
<tr>
<td><strong>TOF-MS</strong></td>
<td>time-of-flight mass spectrometer</td>
</tr>
<tr>
<td><strong>Triple-Quad</strong></td>
<td>triple quadrupole mass spectrometer</td>
</tr>
<tr>
<td><strong>TSRC</strong></td>
<td>Tobacco Science Research Conference</td>
</tr>
<tr>
<td><strong>TUM</strong></td>
<td>Technische Universität München</td>
</tr>
<tr>
<td><strong>UG</strong></td>
<td>University of Gothenburg</td>
</tr>
<tr>
<td><strong>UR</strong></td>
<td>University of Rostock</td>
</tr>
<tr>
<td><strong>VELA</strong></td>
<td>Vehicle emission laboratory</td>
</tr>
<tr>
<td><strong>VOC</strong></td>
<td>volatile organic compounds</td>
</tr>
<tr>
<td><strong>VUV</strong></td>
<td>vacuum ultraviolet</td>
</tr>
<tr>
<td><strong>WELAS</strong></td>
<td>welas® White Light Aerosol Spectrometer</td>
</tr>
<tr>
<td><strong>WSL</strong></td>
<td>Swiss Federal Institute for Forest, Snow and Landscape Research</td>
</tr>
<tr>
<td><strong>WLC</strong></td>
<td>wall loss corrected</td>
</tr>
<tr>
<td><strong>WSOC</strong></td>
<td>water soluble organic compounds</td>
</tr>
<tr>
<td><strong>W-TOF</strong></td>
<td>W-time-of-flight mass spectrometer</td>
</tr>
<tr>
<td><strong>XANES</strong></td>
<td>X-ray absorption near edge structure</td>
</tr>
<tr>
<td><strong>ZAE Bayern</strong></td>
<td>Bavarian Center for Applied Energy Research</td>
</tr>
<tr>
<td><strong>ZAUM</strong></td>
<td>Center of Allergy &amp; Environment</td>
</tr>
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