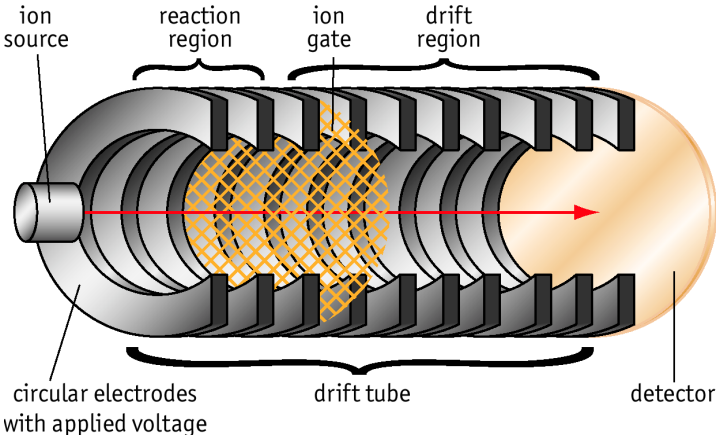
1. IMS-ITMS Ion Mobility Spectrometer Ion Trap Mass Spectrometer

Fears of terrorism and the requirement to detect dangerous chemicals in low concentrations is leading to an ever-increasing need, within homeland security, for reliable, real-time and sensitive detection of a wide range of substances that are a threat to the safety of our society. The chemicals needed to be detected range from explosives through to illegal drugs and chemical and biological warfare agents.

Since 9/11 there has been a significant increase in instrument development to detect explosives (both traditional and homemade) in trace amounts. The most commonly used apparatus for this type of security is often based on the Ion Mobility Spectrometry (IMS). IMS is the underlying technology for a wide range of Chemical Warfare (CW) agent, drug and explosive detectors, and environmental monitors.

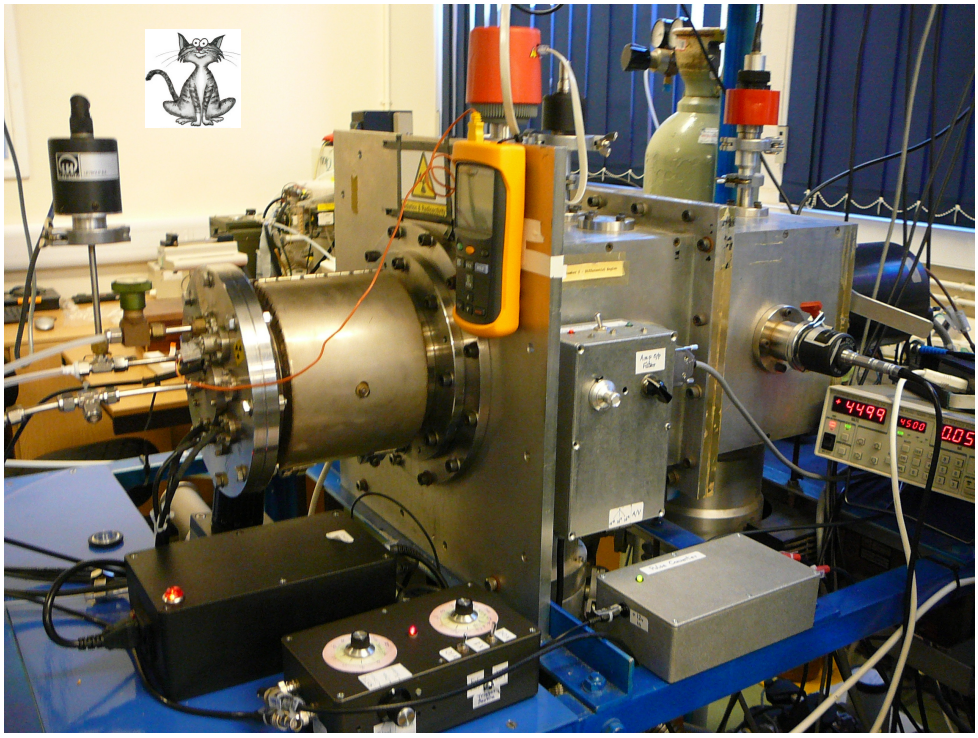


The IMS is constructed of a drift-tube that is made up of a series of rings to create a voltage gradient. A schematic of this set-up is shown below. A carrier gas is introduced, along with the sample and reagent gas into the reaction chamber. Ions are produced in an ion source, which most commonly contains a radioactive source Ni^{63}, within the reaction region. Reactant ions are produced from the reagent gas via a series of reactions with the primary ions. These reactant ions then go onto ionise the sample molecules.

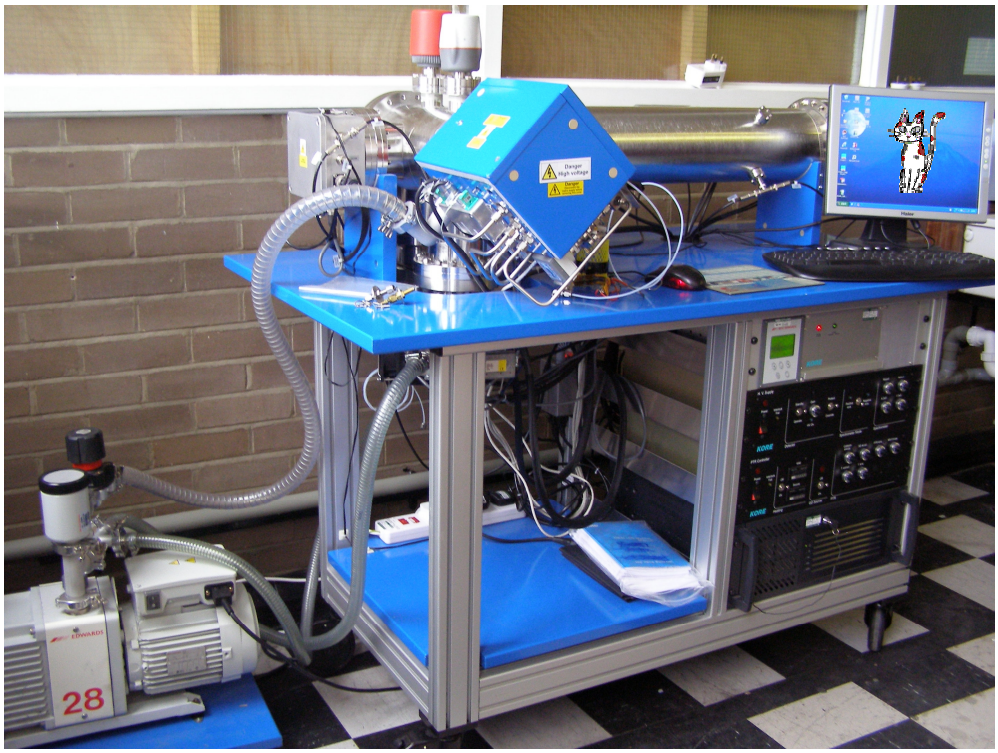
The Molecular Physics group have attached a commercial Ion Mobility Spectrometer (GID-M) from Smiths Detection to an Ion Trap Mass Spectrometer (a Finnigan LCQ Classic). This will provide an insight into the ion chemistry that occurs in an IMS. We are currently studying the ammonia chemistry of the ions produced in the IMS. Future collaborations with Smiths Detection will involve a novel design of Ion Mobility Spectrometer (see the collaborations page).

2. IMS-Quadrupole Mass Spectrometer

The Molecular Physics group also has an IMS-Quadrupole Mass Spectrometer that was built in house, and was adapted from an Electron Attachment system. This is designed to investigate some fundamental ion chemistry that occurs in the IMS and to back up results obtained in the IMS-ITMS system. As it is purely a research instrument, it provides more flexibility of operating conditions and parameters, for example the drift-voltage of the IMS can be altered whereas in the commercial GID-M IMS, it cannot.



3. PTR-TOF-MS Proton Transfer Reaction Time Of Flight Mass Spectrometer



The Department has recently taken delivery of a Kore PTR TOF-MS. This is a versatile Proton Transfer Reaction Time-of-Flight Mass-Spectrometer which is capable of collecting mass spectra in both positive and negative ion mode. We will be using it primarily to look at volatile organic chemicals in the areas of food screening and explosives detection.

Its advantages are that it can capture an entire spectrum in a very short time, there is no upper mass limit and its detection sensitivity is at the parts per billion (volume) level.

4. PTRMS – Proton Transfer Reaction Mass Spectrometer

The Proton Transfer Reaction Mass Spectrometer, PTR-MS is a tool of chemical ionisation mass spectrometry that performs real-time, high sensitivity gas sampling and detection. The PTR-MS was developed by Ionicon, a spin-off company of the University of Innsbruck, Austria. It enables the direct analysis of ambient air or breath samples, with a sensitivity of a few parts per trillion.

The Proton transfer occurs between hydronium ions, H_3O^+ and neutral sample molecules, M:

$$H_3O^+ + M \rightarrow H_2O + MH^+$$

This reaction will occur for neutral molecules with a proton affinity greater than that of water, 691kJ/mol. The major constituent gasses of air have proton affinities below this value, but most volatile organic compounds have proton affinities that allow the reaction to take place. This allows the ambient air of the sample to be used as a buffer in the drift tube.

The air which you exhale from your lungs contains hundreds of VOCs. As a result of various interacting biochemical pathways, not all of which are fully understood by medical science, VOCs are produced which are then released into the blood. From the blood, they can pass through the thin membranes between the capillaries and the alveoli of the lungs, and hence be breathed out. VOCs originating in the body have been identified on the breath at concentrations ranging from below parts-per-billion by volume (ppbv) to parts-per-million by volume (ppmv). Similarly, many drugs and their metabolites will be present on breath at such minute concentrations.

Margaret sampling her breath using the PTR-MS

Many of these VOCs result from normal metabolic processes. However, some of them can be associated with disease states or drug consumption. Breath analysis thus has the potential for disease diagnosis, health status and drug monitoring by "finger-printing" the pattern of trace volatile marker substances in the breath. Of course, some of the VOCs which are detected on the breath may simply be a reflection of the air which has been breathed in. As in so many branches of science, the background must be accounted for.

The potential applications are almost as numerous and wide-ranging as the VOCs themselves. Breath analysis has been investigated in regard to critical care, cardiology, oncology, transplant rejection, renal medicine, respiratory disease, liver disease and infectious diseases, to name but some. The application of the PTR-MS to medicine is of course not just limited to breath analysis, but also to the analysis of emissions from skin (e.g. for the diagnosis of skin cancers), and bodily fluids such as urine.

Through collaborations with colleagues at the Queen Elizabeth Hospital, University Hospital Birmingham NHS Trust, we have already demonstrated the use of the PTR-MS for drug assays and the monitoring of bacterial cultures. We are now planning major clinical trials.

There are many obstacles to overcome with such research, but if successful it could revolutionise diagnosis of disease and drug monitoring. Thus, the PTR-MS and similar instruments based on ion-molecule reactions could become commonplace tools used for the fast diagnosis and monitoring of disease. This would have a major impact on our society.

5. The Selected Ion Flow Tube (SIFT) Apparatus

The SIFT measures the rates and products of bimolecular ion-molecule reactions. This provides useful data on the primary reactions. Positive or negative ions can be created via ionisation by electrons emitted from a hot rhenium filament. The majority of ions are created by a single electron interaction, e.g. N_2^+ and O^-, although there are exceptions, such as H_3O^+ and OH^- which are formed via ion-molecule interactions in the source region. Once created, the ions are focussed into the first quadrupole mass filter region. A quadrupole mass filter is a device which can selectively transmit species with a certain mass/charge ratio. The mass selected ions then form a flowing ion swarm, moving through the flow region in a fast flowing Helium buffer at a pressure of ~ 0.5torr. The ions interact with the reactant molecules introduced into the flow tube, and the parent and product ions are focussed into a second quadrupole mass filter region before detection.