



Project name:

UV analysis of exhaled air

Beamtime Report

17-09-2013 – 24-09-2013 (Date of the report to be added)

General information

Name of the rapporteur	Name of the rapporteur's organisation
Lennart Olsson	Chromalytica AB
Type of research (nanotechnology/health care/chemistry etc.)	Name of the research facility
Health care	Max-Lab
Date of the measurement, duration	Location of the event
17-09-2013 - 24-09-2013	Max-Lab, Lund, Sweden
Facility personnel participating in the measurement	
Mats Leandersson	

Description of the project

Research description (short summary as written in the application)

Exhaled breath comprises thousands of volatile organic compounds (VOCs) of which the composition varies depending on status of the individual and the environment. Different metabolic processes within the body produce volatile substances that are secreted into the blood. When the blood reaches the lungs the products are released into lung tissue and airways. Also, chronic inflammation and/or oxidative stress can result in the excretion of volatile compounds that create distinctive VOC patterns. Therefore, measuring the total amount of VOCs in exhaled air (breathomics), for clinical screening and monitoring reasons has gained increased interest over the last years. The use of individual VOCs as biomarkers of exposure or disease is hindered by the fact that using a single compound is generally inadequate to monitor complex and heterogeneous processes including environmental exposures or chronic diseases. Therefore, exploring the total amount of exhaled VOCs, called the volatome, is expected to create more relevant information regarding the processes involved. Indeed, analyzing the volatome implies a more specific discrimination between various conditions as it reflects changes in both exogenous and endogenous compounds. One technique that allows for the detection of the volatome is Gas Chromatography-Deep Ultraviolet Spectroscopy (GC-DUV). It has been used both for the valuation of environmental factors as well as for individual VOCs. However, its use has been hampered by its technical design.

Recently, Chromalytica AB has developed a new GC-DUV (figures 1-2) with a dedicated charged coupled device (CCD).

In UV spectroscopy, the sample is irradiated with the broad spectrum of the UV radiation. If a particular electronic transition matches the energy of a certain band of UV, it will be absorbed. The remaining UV light (residual radiation) passes through the







sample. From this residual radiation an absorption spectrum is obtained (figure 3). Traditionally, deuterium light sources have been and are used, but many have an uneven spectral distribution that needs to be taken into consideration when selecting the appropriate charged coupled device (CCD), detector. Also, the functioning of CCDs in the vacum region (below 200 nm) is not well known.

The aim of our investigation was to elucidate the properties of the Chromalytica AB's CCD, using a beam with a selective spectral distribution.

Summary of activities (experiments performed, beamtime used, preliminary overview of results, next steps and other relevant information)

In the present set of experiments, carried out at Max-Lab using the beam at MAX III, we studied the properties of our CCD as well as its detection limits. Utilising the accuracy of the UV radiation at the I3 beamline at MAX III it was clearly demonstrated, for the first time, that the CCD used by Chromalytica has a detection capacity below 160 nm (figure 4). As shown there is a first (153 nm) and second (306 nm) harmonics from the CCD while using a beam with a wavelength of 153 nm. The relatively large signal from the second harmonic in comparison to the first harmonic indicated that the CCD needed adjustments.

In the present modified Chromalytica AB unit, developed after the tests at Max-Lab, the CCD has been adjusted and the second harmonics abolished allowing for a better and more specific analysis. The shortcomings of the CCD set up, discovered at Max-Lab, has allowed for important adjustments – adjustments that would not possible without having the CCD tested at MAX III.

How would you describe cooperation and assistance from industrial liaison officers and national contact points while preparing and carrying out the research at large scale facilities?

Beam time was well used after a relatively fast set up with alignment using dedicated holders made by Max-Labs personnel in their workshop. From our point of view we had an excellent support with very enthusiastic personnel. We could not wish for better!

Other personal remarks

Thanks to MAX-Lab and the decision of Science Link to accept Chromalytica ABs application as a user of the facilities at MAX III we obtained results which were of significant importance for our further development.

The Max-Lab initiative shows how science based set ups may foster the development and the support of novel companies and techniques. Without the opportunity given to Chromalytica AB to participate, the technique now used by us would not have been developed.







<u>Annexes</u>

Annexes (list of annexes; meeting minutes, graphical illustrations, tables and other supplementary data)

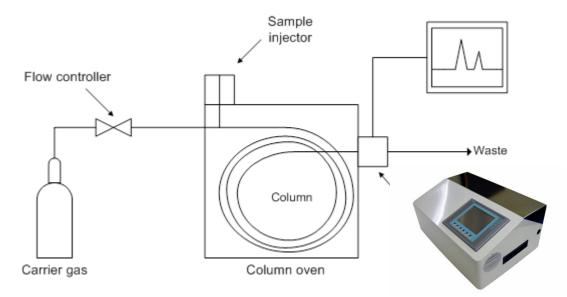


Figure 1. Schematic illustration of the Chromalytica GC-DUV instrumentation.



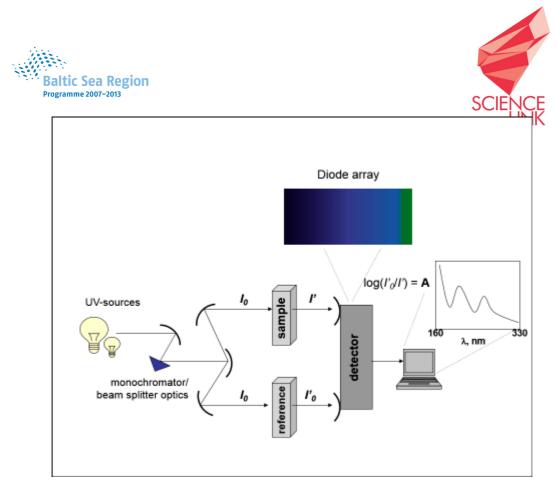


Figure 2. Schematic presentation of the principles of GC-DUV spectroscopy.

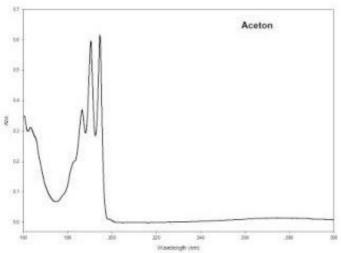


Figure 3. The UV-vis spectrum of Aceton. The presence of Aceton in exhaled air is an indication of diabetes.







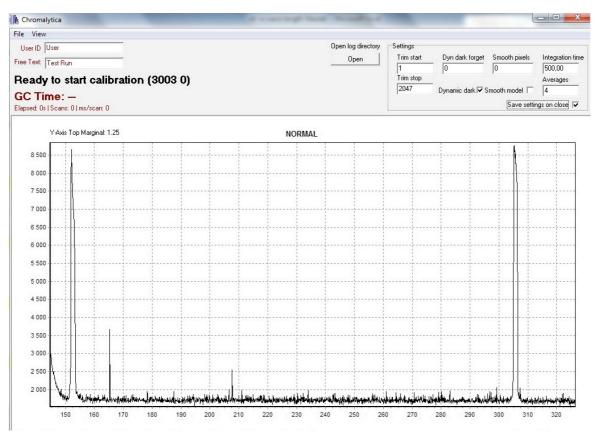


Figure 4. Spectrum achieved by scanning the UV region with the monochromator (no VOCs). The beam was set to153 nm.

