Environmental Analysis of Air, Water, and Soil using LDTD-APCI MS/MS

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Introduction

Rapid on-site chemical analysis is very important to evaluate potential environmental contaminations from chemicals and accidental chemical spills. In such situations, accurate and timely information on the types and level of toxic chemicals is required to prevent the public exposition from these chemicals. For real-time, direct-air sampling and for fast water and soil analysis, the LDTD-APCI MS/MS system is used.

Goals

- Illustrate the efficiency of the LDTD-APCI source for air analysis;
- Develop an easy gas calibration procedure and;
- Demonstrate the capacity of the LDTD-APCI MS/MS system for water and soil samples analysis.

Instrumentations

- Phytronix Technologies LDTD ionization source (model T-960);
- Thermo Scientific TSQ® Quantum™ Ultra AM mass spectrometer.

LDTD-APCI MS/MS system for Air Analysis

On-line air sampling is performed from an aerial sampling probe by a sampling pump controlled by a mass flow controller which provides accurate flow over normal atmospheric condition variations (pressure and temperature). The regulated air flow is introduced into the transfer tube and into a corona discharge region where APCI of the gas molecules is initiated. The produced ions are then introduced into the mass spectrometer for analysis. The LazSoft™ software controls the LDTD-APCI source and the air sampling pump. It also displays and archives data from the weather station. The LDTD-APCI MS/MS system is installed on a damping table to prevent vibrations during real-time data acquisition while traveling through contamination site.

Gas Calibration Procedure

Concentration calibration is performed using a gas tight syringe pump system. Continuous air is introduced into the gas flow system (up to 10 L/min) at incremental flow values to generate different gas concentrations.

For ultra low concentration calibration, certified gas cylinder are sampled and diluted into a 10 L/min air flow and introduced into the LDTD-APCI source. A mass flow controller is used to control the sampling flow and allows gas concentration to be adjusted.

Water and Soil Analysis

The LDTD-APCI source is equipped with a bar coded LazWell™ plate (96-well plate) to introduce liquid samples for water analysis or soil extract from liquid-liquid extraction. The liquid sample, dried at TPN onto a well, is thermally desorbed indirectly by a infrared laser diode. The gas phase molecules are then carried over by a carrier gas into the APCI region and the produced ions are transferred into the mass spectrometer.

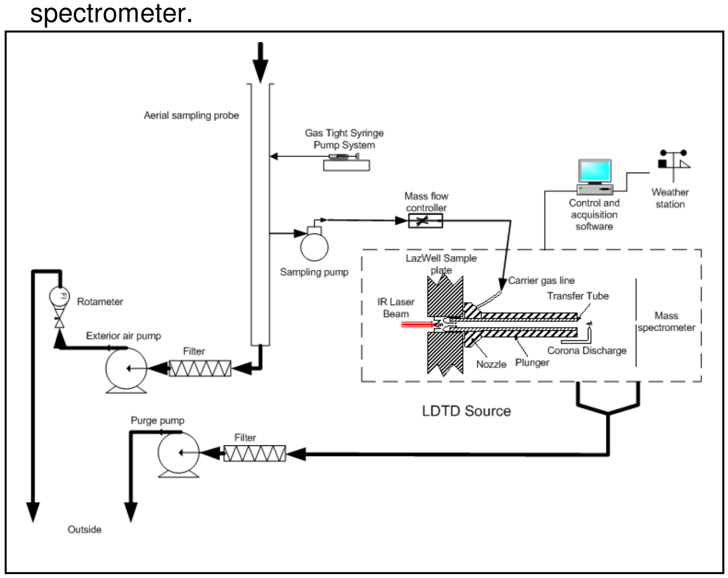
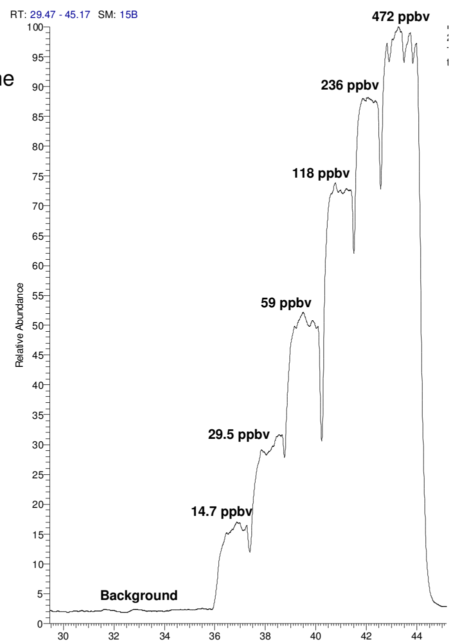


Figure 1 Schematic representation of the LDTD-APCI MS/MS for on-line air analysis. The system also performed water and soil extract analysis.

Results and Discussions

Accurate air analysis is allowed with the LDTD-APCI source using the calibration procedure (gas tight syringe pump system). Incremental concentration step produced stable toluene signal (**Fig. 2**). From the toluene calibration curve obtained in MS/MS (**Fig. 3**), the analytical LOD is 0.2 ppbv and the LOQ is 0.7 ppbv. These values are typical LOD and LOQ obtained with the LDTD-APCI source for gaseous compounds.

Figure 2 Low concentration calibre-tion spectra for Toluene analysis in Air.



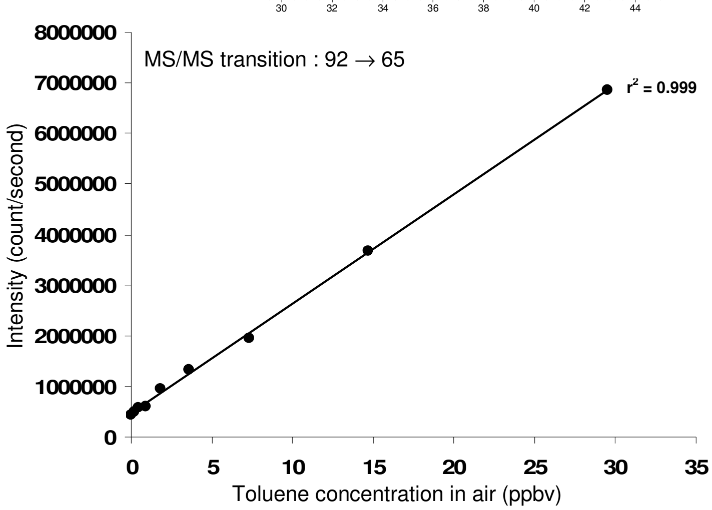


Figure 3 Low calibration curve for atmospheric Toluene analysis using the LDTD-APCI source

To illustrate the LDTD-APCI source potential, several gaseous compounds have been detected and quantified in negative APCI (Acetic acid, Cyanidric acid and n-Phenol) and positive APCI (CS_2, NH_3, Acetonitrile, Acetone, Dichloromethane, Methanol, Ethanol, n-Butyraldehyde, hexane, Cyclohexanone, n-Amyl acetate, and Diisopropyl methylphosphonate) (e.g. **Figs. 4, and 5**).

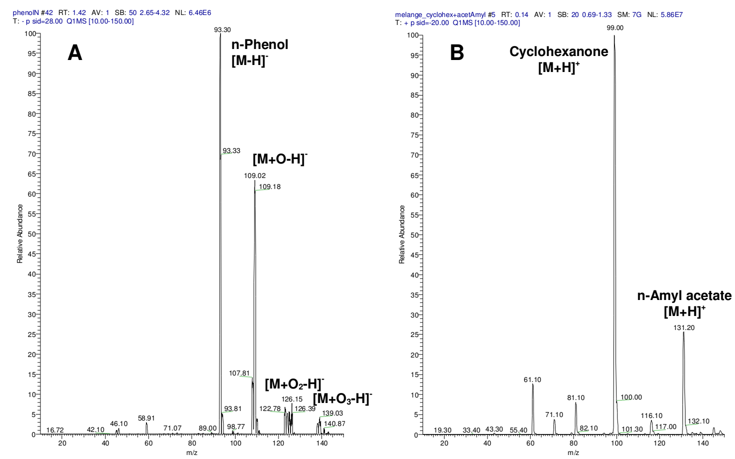


Figure 4 Air analysis of n-Phenol in negative LDTD-APCI (**A**), and of a air mixture of Cyclohexanone and n-Amyl acetate in positive LDTD-APCI (**B**).

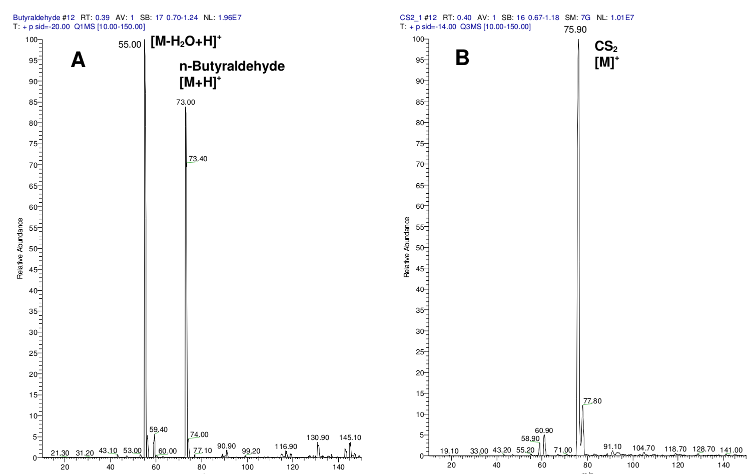


Figure 5 Positive LDTD-APCI MS/MS analysis of n-Byturaldehyde (**A**) and CS_2 (**B**) in air.

Soil and water may also be contaminated following accidental chemical spills. As example, the LazWell™ plate is used to perform soil extract analysis with the LDTD-APCI source. A classic liquid-liquid sample extraction procedure is performed on a contaminated soil and Hexachlorobenzene (C_6Cl_6) was detected. The negative LDTD-APCI spectrum is shown in **Figure 6**.

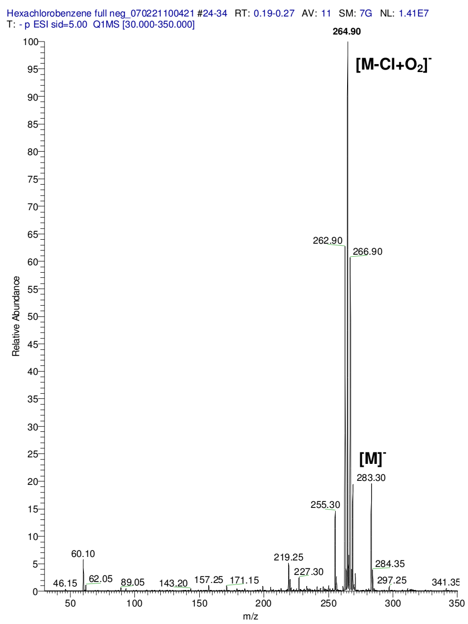


Figure 6 Soil extract analysis of Hexachlorobenzene in negative LDTD-APCI.

Conclusion

The LDTD-APCI source has been successfully operated in a mobile laboratory for environmental analysis. The LDTD-APCI technology allows fast mass spectrometric analysis without extensive sample preparation. Atmospheric pollutants could easily be detected and quantified in the low ppbv concentration range. Water and soil extract analysis can also be performed with the system. The LDTD-APCI MS/MS system performs direct on-line analysis of air and also manages liquid samples for a complete on-site environmental evaluation. The LDTD-APCI source is the only one on the market allowing such possibilities in environmental analysis.

References

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