FT-IR spectroscopy & Machine Learning for highly ultrasensitive detection and discrimination of Volatile Organic Compounds

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Volatile Organic Compounds (VOCs), such as styrene and its co-products, are organic chemical compounds able to evaporate at room temperature. They are classified as a possible human carcinogen in the short and long term and in co-exposure to other physical-chemical agent. Several gold standard methods exist for their detection in the atmosphere; however, most of them operate ex-situ or do not provide easy discrimination between different molecules with limited sensitivity.
During the last years, in the framework of the strong collaboration with University Roma Tre and INAIL, we systematically used Fourier Transform Infrared (FTIR) spectroscopy for quantifying VOCs in air, increasing the sensitivity of IR systems down to the parts per million (ppm) level, promising starting point for building a portable setup for the detection at very high sensitivity
In this presentation, we introduce an improved and ultrasensitive method based on Fourier Transform Infrared (FTIR) spectroscopy to analyze toxic gaseous substances with the aim of filling the gap in IR gas-phase database of universal and unique calibration curves. We investigate nine selected aromatic compounds of extreme importance in occupational safety. To provide the automatic recognition method for VOCs, we propose Machine Learning (ML) based methods, such as Support Vector Machines, K-Nearest Neighbours, and Random Forests, for identification and classification of them through using the IR gas-phase database.