Analysis of toxic substances by gas chromatography/multiphoton ionization/time-of-flight mass spectrometry

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Abstract of Dissertation

In this dissertation, I have developed a new analytical tool to detect toxic substances, which is based on gas chromatography combined with multiphoton ionization time-of-flight mass spectrometry (GC/MPI/TOF-MS). This dissertation is divided into five chapters as follows.

Chapter 1 outlines a brief introduction on the effect of organochlorine pesticides to environment. Further, the risk of psycho active substances on public health is also explained. To address the environmental effects as well as public health risks, it is important to analyze pesticides and drugs selectively. Therefore, a new analytical technique is required to achieve this purpose. Chapter 1 further explains the principles of GC/MPI/TOF-MS.

Chapter 2 outlines a strategy used to analyze thirteen organochlorine pesticides by gas chromatography combined with mass spectrometry using an ultraviolet femtosecond laser (267 nm) as an ionization source. When an ultrashort optical pulse was used for ionization, molecular ions were typically produced which was preferential for reliably identifying the analytes. The ionization mechanism was studied based on three models constructed for resonance-enhanced two-photon ionization, non-resonant two-photon ionization, and non-resonant three-photon ionization. The results in this study suggest that two-photon ionization with minimum excess energy would be optimal for observing a molecular ion.

Chapter 3 outlines a strategy used to suppress fragmentation of *cis*- and *trans*-methyl cyclohexanols. Suppressing fragmentation is a constant challenge in mass spectrometry, since a molecular ion can readily be identified and provides information concerning the molecular weight of an analyte. We report on the use of tunable ultraviolet (UV) and near-infrared (NIR) femtosecond lasers (35 fs) for the multiphoton ionization (MPI) of 4-methylcyclohexanols, the reference molecules

that are currently used to examine fragmentation suppression. The results were compared with those obtained by charge exchange chemical ionization (CECI) and vacuum ultraviolet emission ionization (VUVEI), since they were reported as the best techniques for suppressing fragmentation. A molecular ion was strongly enhanced by carefully minimizing the excess energy in the ionic state using tunable UV and NIR lasers. The ratio of the intensities for molecular and fragment ions, increased significantly compared to the values obtained by CECI and VUVEI, respectively.

Chapter 4 outlines a strategy used to suppress a cleavage of a chemical bond between the α- and β-carbons in amino related psycho active substances using a UV femtosecond laser emitting at different laser wavelengths. As a result, dominant fragmentation appeared in electron ionization was significantly suppressed for some of the psychoactive substances. Chapter 4 further discusses possible fragmentation pathways of psycho active substances using GC/MPI/TOF-MS.

Chapter 5 explains the general summery of the thesis with perspectives on future works.