Fiche résumé

❖ Sujet de la recherche :

Evaluation of different vibrationnal activation modes for fast isomeric organophosphonate distinction

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❖ Résumé des travaux et principaux résultats obtenus :

Despite the ratification of Chemical Weapon Convention (CWC) by the majority of countries all around the world, chemical warfare agents, like organophosphorus compounds, remain a potential threat to both health and environment. Nerve gases are readily hydrolyzed in water and produce characteristic alkyl phosphonate and analog compounds. The detection of degradation products gives indirect evidence of a nerve gas presence. All these compounds are listed in the CWC. A particular challenge is the structural elucidation of the side alkyl chain bounded to phosphorus atom of the CWA compounds or after partial or total degradation under the natural ambient, or after decontamination. Under low energy CID conditions, the very labile O-alkyl chain of protonated alkyl phosphonic acids or alkyl alkylphosphonate compounds, is regioselectively disrupted. Indeed, only these protonated O-C bond competitive cleavages are observed and more rarely the P-C bond rupture, which is very stable. The aim of our work was to provide a direct method favoring fast consecutive processes able to generate the diagnostic m/z 83 product ion in only one step from precursor ion. Such way should be also consistent with the OPCW laboratory rules which required, under API conditions, one MS² experiment from the intact precursor ion characterizing the samples, e.g., the m/z 211 ion for the O-Ethyl O-Methoxyethyl isopropylphosphonate. To reach this objective, several ion activation methods were explored (e.g., resonant and non resonant CID, SORI-CID and IRMPD) using FTMS instruments (Qh-FTICR and LTQ-Orbitrap) as well as low resolution instruments (quadrupole ion trap and triple quadrupole).

The need of activation techniques which activated both m/z 211 precursor ion and its m/z 125 product ion was required due to the high and quick cooling rate of product ions in a quadrupole ion trap at a pressure about 10⁻⁵ mBar. Actually, in this case; only the isopropyl isomer leaded to the m/z 83 diagnostic ion. Nevertheless, the resonant CID experiments realized on the ICR cell, at ultra vacuum, leaded to differentiation of the two O-alkyl propylphosphonate isomers in one step. Some m/z 107 abundance differences were also observed between the two isomers. This observation was probably explained by the competitive fragmentation pathways in the case of the iso-propyl isomer contrary to the n-propyl isomer where the P-alkyl chain loss was disadvantaged compared to the water loss.

❖ Perspectives envisagées

These activation modes could be used for different isomer phosphonate compounds. The next step is to test them to analyse complex mixtures.