Researchers provide new information about mass spectrometry

October 15 2007

Fresh data on mass spectrometry are presented in the report ‘Low-energy collision-induced fragmentation of negative ions derived from ortho-, meta-, and para-hydroxyphenyl carbaldehydes, ketones, and related compounds,’ produced by Professor Athula Attygalle and his colleagues in the Center for Mass Spectrometry at Stevens Institute of Technology.

According to a study, “Collision-induced dissociation (CID) mass spectra of anions derived from several hydroxyphenyl carbaldehydes and ketones were recorded and mechanistically rationalized. For example, the spectrum of m/z 121 ion of deprotonated ortho-hydroxybenzaldehyde shows an intense peak at m/z 93 for a loss of carbon monoxide attributable to an ortho-effect mediated by a charge-directed heterolytic fragmentation mechanism.”

“In contrast, the m/z 121 ion derived from meta and para isomers undergoes a charge-remote homolytic cleavage to eliminate an *H and form a distonic anion radical, which eventually loses CO to produce a peak at m/z 92. In fact, for the para isomer, this two-step homolytic mechanism is the most dominant fragmentation pathway. The spectrum of the meta isomer on the other hand, shows two predominant peaks at m/z 92 and 93 representing both homolytic and heterolytic fragmentations, respectively. (18)O-isotope-labeling studies confirmed that the oxygen in the CO molecule that is eliminated from the anion of meta-hydroxybenzaldehyde originates from either the aldehydic or the phenolic group. In contrast, anions of ortho-hydroxybenzaldehyde and 2-hydroxy-1-naphthaldehyde, both of which show two consecutive CO eliminations, specifically lose the carbonyl oxygen first, followed by that of the phenolic group. Anions from 2-hydroxyphenyl alkyl ketones lose a ketene by a hydrogen transfer predominantly from the alpha position. Interestingly, a very significant charge-remote 1,4-elimination of a H(2) molecule was observed from the anion derived from 2,4-dihydroxybenzaldehyde," wrote Attygalle and his colleagues from Stevens.

The researchers concluded: "For this mechanism to operate, a labile hydrogen atom should be available on the hydroxyl group adjacent to the carbaldehyde functionality."

Attygalle and colleagues published the results of their research in the *Journal of Mass Spectrometry* (Low-energy collision-induced fragmentation of negative ions derived from ortho-, meta-, and para-hydroxyphenyl carbaldehydes, ketones, and related compounds.

Citation: *Journal of Mass Spectrometry*, 2007; 42(9):1207-17).

Source: Stevens Institute of Technology

Citation: Researchers provide new information about mass spectrometry (2007, October 15) retrieved 24 April 2024 from https://phys.org/news/2007-10-mass-spectrometry.html