



Investigations of the fragmentation pathways of benzylpyridinium ions under ESI/MS conditions

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Auteur	Zins, Emilie-Laure [1], Rondeau, David [2], Karoyan, Philippe [3], Fosse, Céline [4], Rochut, Sophie [5], Pepe, Claude [6]
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Résumé en anglais	<p>Benzylpyridinium ions are often used as 'thermometer ions' in order to evaluate the internal energy distribution of the ions formed in sources of mass spectrometers. However, the detailed fragmentation pathways of these parent ions were not well established. In particular, fragmentation involving a rearrangement (RR) process may be influencing the simulated distribution curves. In a previous study, we suggested that such RR actually occurred under electrospray ionization/mass spectrometry (ESI/MS) and fast atom bombardment/mass spectrometry (FAB/MS) experiments. Here, we present a systematic study of different substituted benzylpyridinium ions. Theoretical calculations showed that RR fragmentation leading to substituted tropylium ions could occur under 'soft ionization' conditions, such as ESI or FAB. Experimental results obtained under gas-phase reactivity conditions showed that some substituted benzylpyridinium compounds actually undergo RR fragmentations under ESI/MS conditions. Mass-analyzed kinetic experiments were also carried out to gain information on the reaction pathways that actually occur, and these experimental results are in agreement with the reaction pathways theoretically proposed.</p>
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