Saccharose: Sweet and Ubiquitous Mass Calibrant for Direct Analysis in Real Time—Fourier Transform Ion Cyclotron Resonance—Mass Spectrometry

Jürgen H. Gross
Institute of Organic Chemistry, Heidelberg University, Im Neuenheimer Feld 270, 69120 Heidelberg, Germany

Project

- In positive-ion direct analysis in real time mass spectrometry (DART-MS) [1] mono-, di-, and tri saccharides all form \( [M+NH_4]^+ \) ions.
- Some of them, in addition, yield abundant \( [M+2NH_4]^+ \) cluster ions [2].
- Highly polar or ionic analytes commonly deliver cluster ion series that extend to high mass [3], and thus, may serve for mass calibration [4].
- Saccharose, the most common sugar, is among the \( [M+NH_4]^+ \) cluster ion forming species.
- Saccharose may therefore be employed as a mass calibration standard.
- The extent of saccharose cluster ion formation depends on the temperature of the DART gas, sample load, and instrumental parameters like trapping conditions of ions prior to mass analysis.
- This study identifies optimized experimental conditions and presents illustrative applications of saccharose cluster ion based mass calibration for accurate mass measurements in DART—FT—ICR—MS.

Conclusions

- In positive-ion DART-MS saccharose yields \( [M+NH_4]^+ \) cluster ions.
- Saccharose cluster ion formation depends on the temperature of the DART gas, sample load, trapping gas pressure, and instrumental factors.
- For best cluster ion formation, experimental conditions need to be well defined.
- Cluster ions of saccharose can be exploited as a cheap and ubiquitous means for DART mass calibration.

References


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These spectra were obtained using a mass calibration based on saccharose cluster ions. In positive-ion DART, DEHP, a common polymeric impurity, forms \( [M+H]^+ \) ions, polyvinylpyrrolidone yields \( [M^+ \cdot 2NH_4]^+ \) as well as more abundant \( [M+NH_4]^+ \) ions, and silicone oil (PDMS) also preferentially yields \( [M+NH_4]^+ \) ions. The accurate mass results from four repetitive runs are tabulated below.

With the given instrumentation, a standard deviation of < 2 ppm may be achieved.

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Conference Contributions.