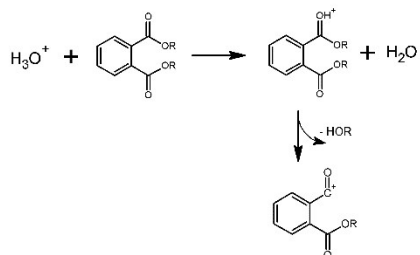


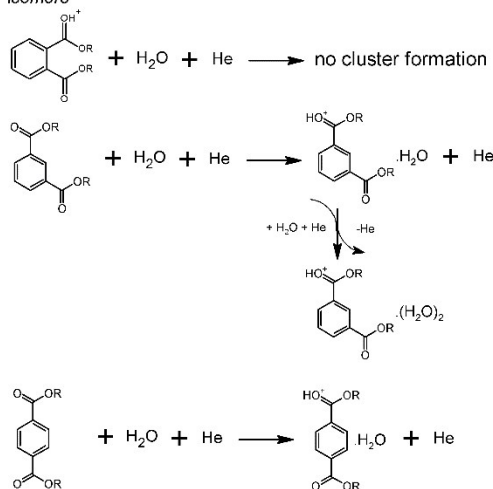
## Ion chemistry of phthalates in selected ion flow tube mass spectrometry: isomeric effects and secondary reactions with water vapor

M. Lacko,<sup>a,b</sup> B. Michalczuk,<sup>c</sup> Š. Matejíček<sup>c</sup> and P. Španěl<sup>a</sup>

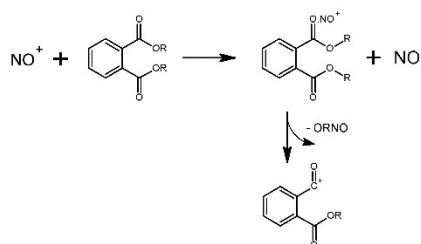
Primary reaction with  $\text{H}_3\text{O}^+$



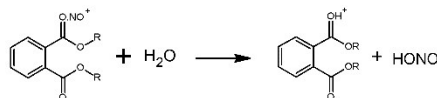
Secondary reaction with  $\text{H}_2\text{O}$  - only for DMP meta and para isomers



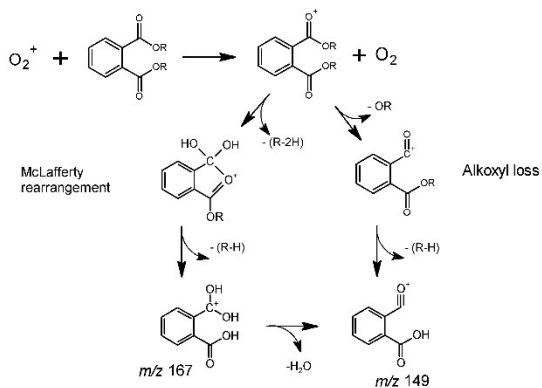
Primary reaction with  $\text{NO}^+$



Secondary reaction with  $\text{H}_2\text{O}$



Primary reaction with  $\text{O}_2^+$



Scheme S1: Mass spectrum of DBP using  $\text{H}_3\text{O}^+$  reagent ions. Selected peaks presented during the direct sampling of DPB headspace are not related to the DBP ion chemistry.

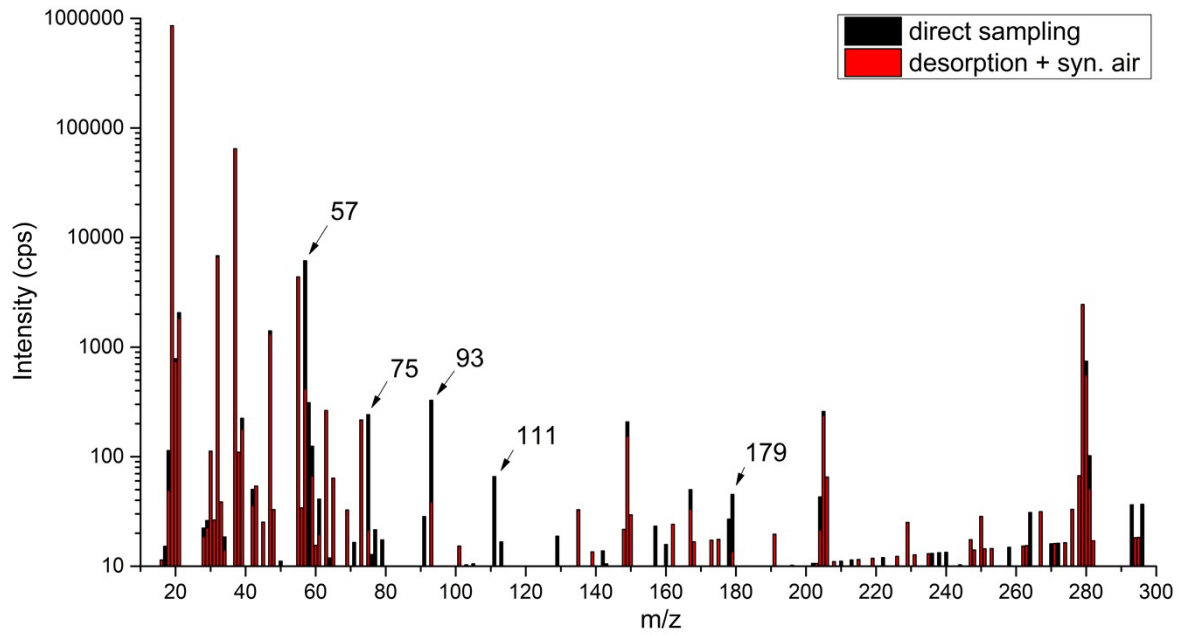


Figure S1: Mass spectrum of DBP using  $\text{H}_3\text{O}^+$  reagent ions. Selected peaks presented during the direct sampling of DPB headspace are not related to the DBP ion chemistry.

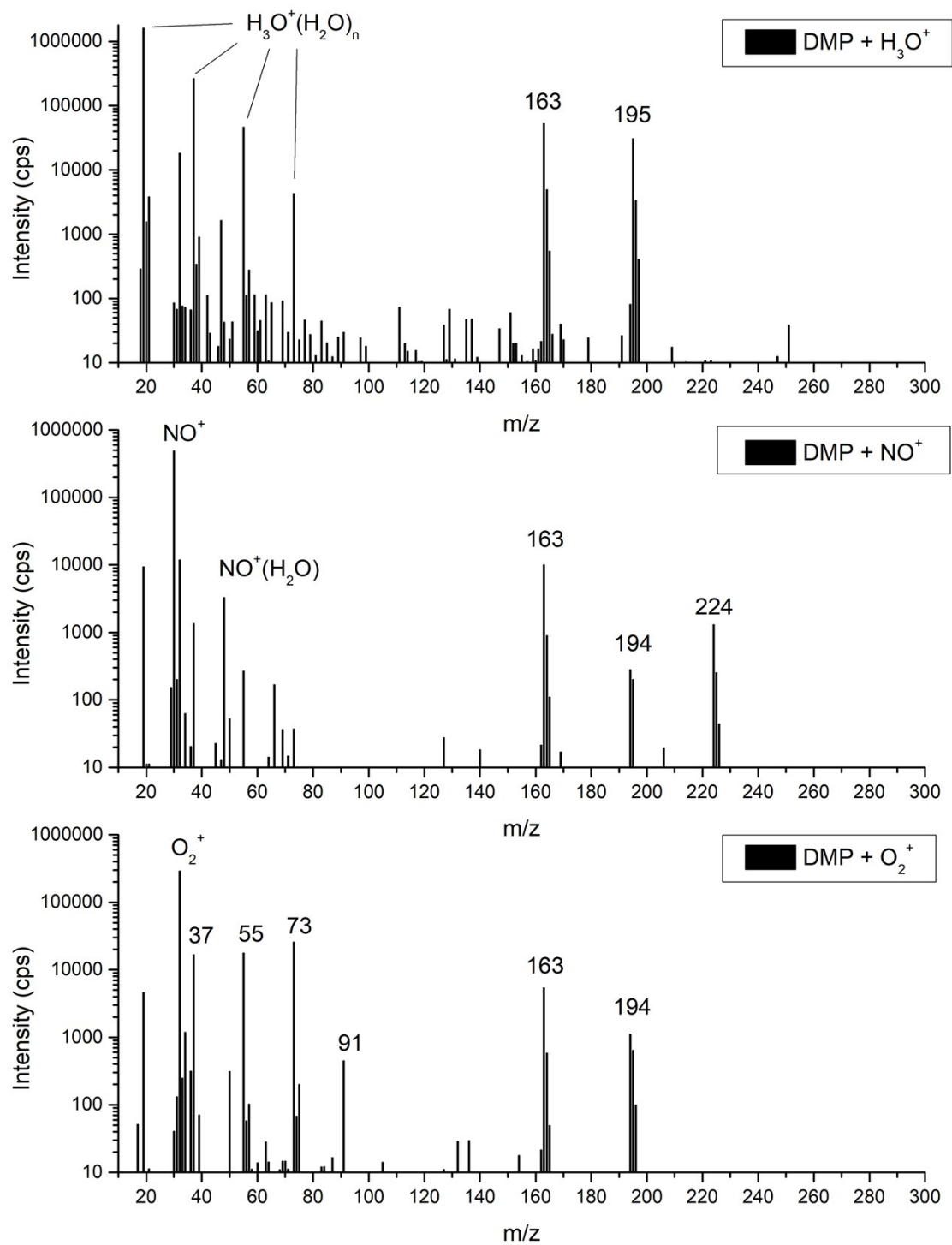


Figure S2: Mass spectrum of DMP using H<sub>3</sub>O<sup>+</sup>, NO<sup>+</sup> and O<sub>2</sub><sup>+</sup> reagent ions.

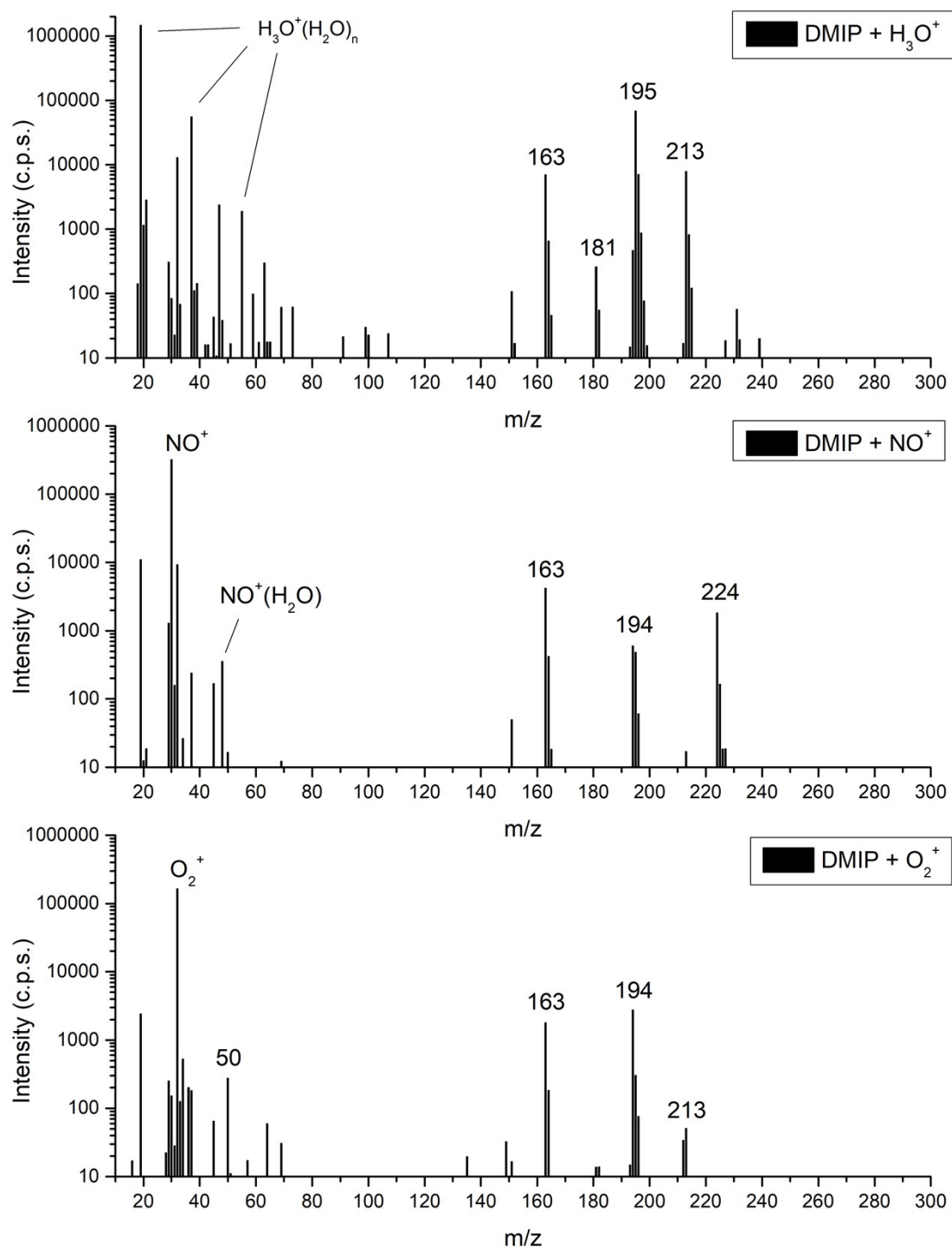


Figure S3: Mass spectrum of DMIP using H<sub>3</sub>O<sup>+</sup>, NO<sup>+</sup> and O<sub>2</sub><sup>+</sup> reagent ions.

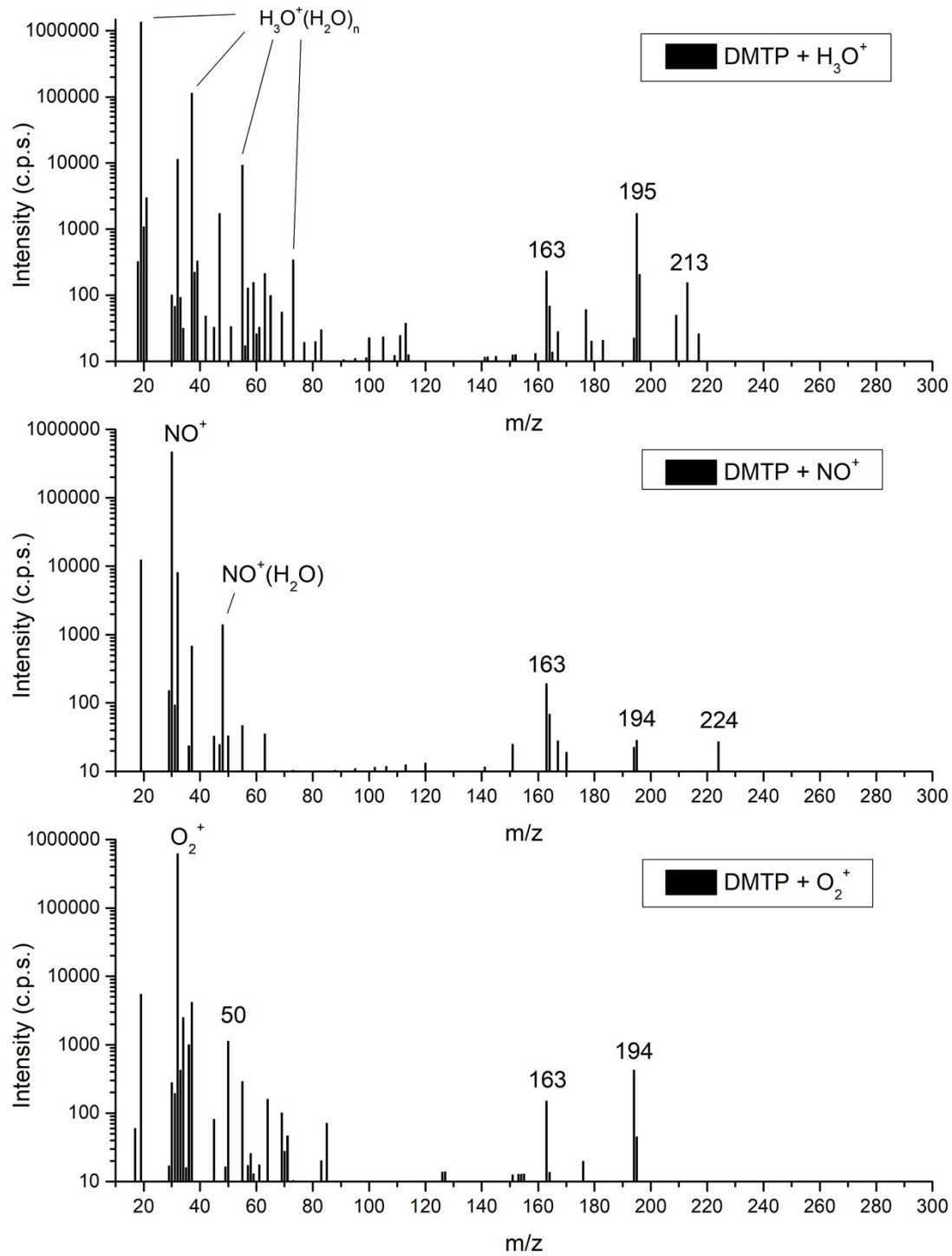


Figure S4: Mass spectrum of DMTP using  $\text{H}_3\text{O}^+$ ,  $\text{NO}^+$  and  $\text{O}_2^+$  reagent ions.

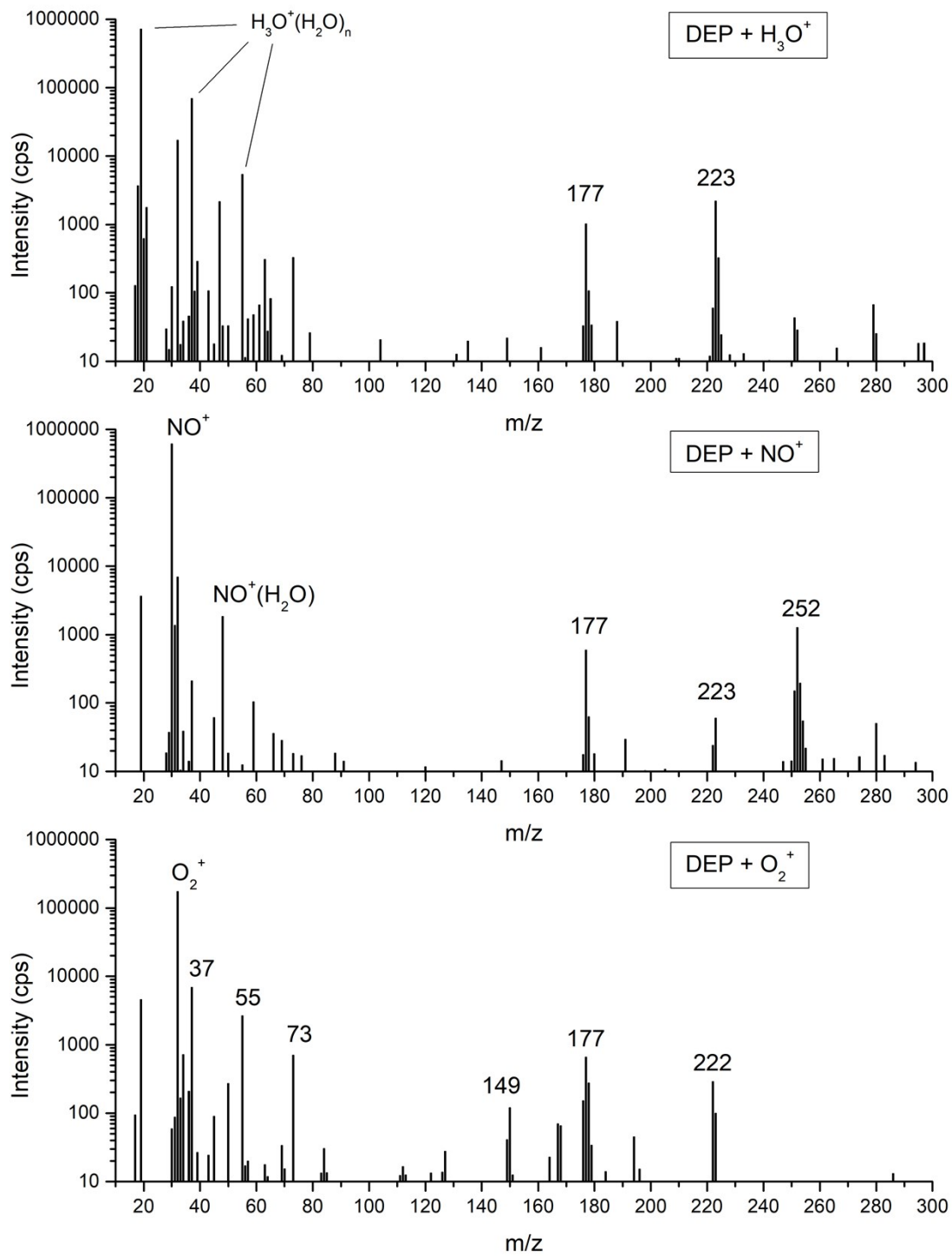


Figure S5: Mass spectrum of DEP using H<sub>3</sub>O<sup>+</sup>, NO<sup>+</sup> and O<sub>2</sub><sup>+</sup> reagent ions.

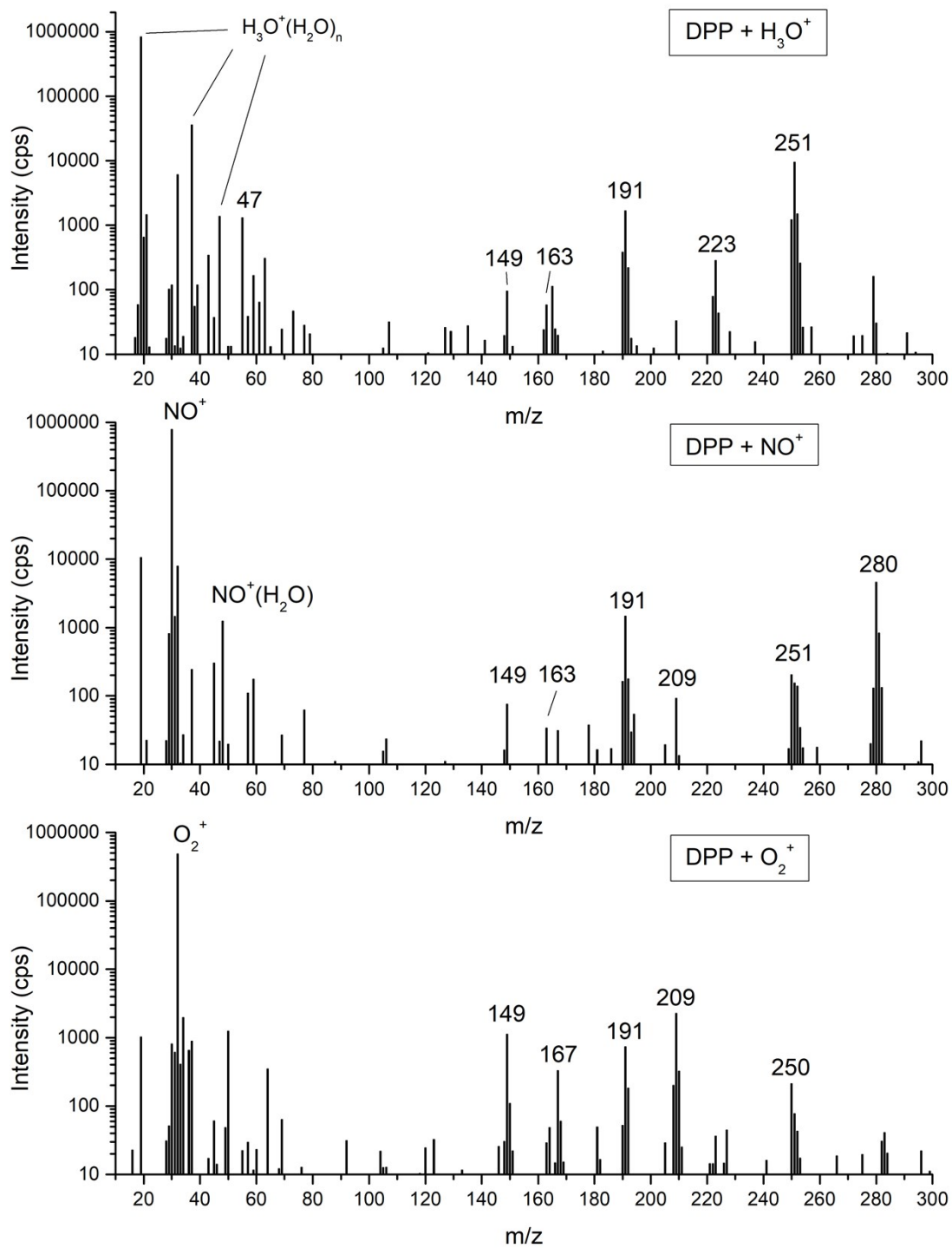


Figure S6: Mass spectrum of DPP using H<sub>3</sub>O<sup>+</sup>, NO<sup>+</sup> and O<sub>2</sub><sup>+</sup> reagent ions.

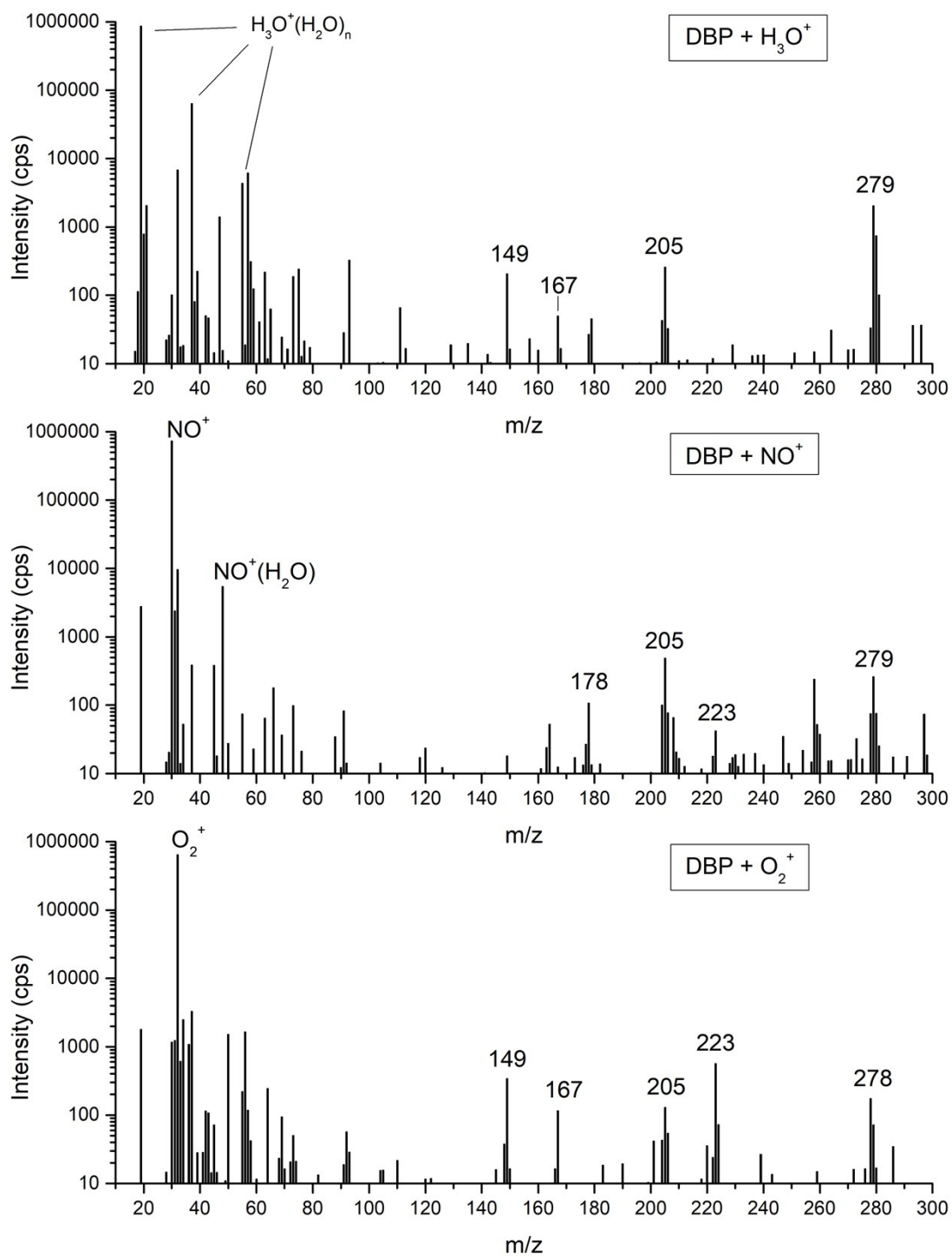


Figure S7: Mass spectrum of DBP using H<sub>3</sub>O<sup>+</sup>, NO<sup>+</sup> and O<sub>2</sub><sup>+</sup> reagent ions.