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Stability of proton-bound clusters of alkyl alcohols, aldehydes and ketones in Ion Mobility Spectrometry

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ABSTRACT

Significant substances in emerging applications of ion mobility spectrometry such as breath analysis for clinical diagnostics and headspace analysis for food purity include low molar mass alcohols, ketones, aldehydes and esters which produce mobility spectra containing protonated monomers and proton-bound dimers. Spectra for all n- alcohols, aldehydes and ketones from carbon number three to eight exhibited protonated monomers and proton-bound dimers with ion drift times of 6.5 to 13.3 ms at ambient pressure and from 35 to 80 ºC in nitrogen. Only n-alcohols from 1-pentanol to 1-octanol produced proton-bound trimers which were sufficiently stable to be observed at these temperatures and drift times of 12.8 to 16.3 ms. Polar functional groups were protected in compact structures in *ab initio* models for proton-bound dimers of alcohols, ketones and aldehydes. Only alcohols formed a V-shaped arrangement for proton-bound trimers strengthening ion stability and lifetime. In contrast, models for proton-bound trimers of aldehydes and ketones showed association of the third neutral through weak, non-specific, long-range interactions consistent with ion dissociation in the ion mobility drift tube before arriving at the detector. Collision cross sections derived from reduced mobility coefficients in nitrogen gas atmosphere support the predicted ion structures and approximate degrees of hydration.

Keywords: proton-bound trimers, aldehydes, n-alcohols, ketones, ion mobility spectrometry, molecular modeling.

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