Generation of negative ion mobility standards using tetra-alkyl ammonium halide salts

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Tetra alkyl halide salts, dissolved in high grade alcohols as reviewed by Ude & Fernández de la Mora (2005) have proven to be very good candidates for the generation of positively charged, well defined molecular clusters. Definitely, it can be said, that the possibility of the generation of ion mobility standards has opened the doors for new ways of generating test/model aerosols for laboratory experiments and for instrument calibration.
In positive mode, the mobility distribution of tetra-alkyl ammonium halide salts yields a unique pattern of peaks, associated with stable cluster species of the form $A^+(AB)_n$, where "A" denotes the tetra-alkyl ammonium ion (monomer) and "AB" the neutral tetra-alkyl ammonium halide molecule.

In this work, tetra alkyl ammonium halide salts are used to generate the negatively charged counterpart-clusters of the positive mobility standards. Accordingly, the cluster can be described in the form $A^-(AB)_n$, where "A" denotes the negatively charged halide ion, and "AB" again the neutral tetra-alkyl ammonium halide molecule, as observed by Kangasluoma et al. (2013).

The negatively charged clusters are produced by means of an electrospray generator (ES). The version used in this study is a slightly modified version of the design presented by Rosell-Llompart and Fernández de la Mora (1994). The redesign features an improved observation of the interior of the electrospray chamber with an inbuilt LED light source and an optical system with a high resolution microscope camera (3 mega pixel). The mobility analysis of the ion clusters was performed with a newly developed high resolution mobility analyzer (UDMA; Steiner et al. 2010), running in a closed-loop configuration to avoid unwanted contaminations.

For the preliminary experiments, four different tetra-alkyl halide salts where used:

- tetra-ethyl ammonium chloride (TEACl)
- tetra-butyl ammonium iodide (TBAI)
- tetra-pentyl ammonium iodide (TPAI)
- tetra-heptyl ammonium bromide (THABr)

For TBAI, TPAI and THABr, spectroscopy grade methanol was chosen as solvent liquid, TEACl was dissolved in spectroscopy grade acetonitrile. For every substance, a base-solution of 1mMol/L was made. If necessary, the base solution was further diluted to increase the signal intensity of the clusters. Carrier gases where purified compressed air or synthetic air from a gas cylinder.

The results displayed in Figure 1 show sharp peaks for every substance, associated to the dimer and trimer clusters of the negatively charged tetra-alkyl halides. Since the ES is operated at relatively high voltages between 3 to 4kV, ions originating from a corona discharge on the tip of the capillary are observed. Therefore, unfortunately no mobility/size peak of the monomer clusters (the negative halide ion) can be separated.

For future experiments, it is planned to setup the high resolution UDMA in series to a mass spectrometer, for a mass-to-charge analysis and chemical identification of the generated molecular ion clusters.

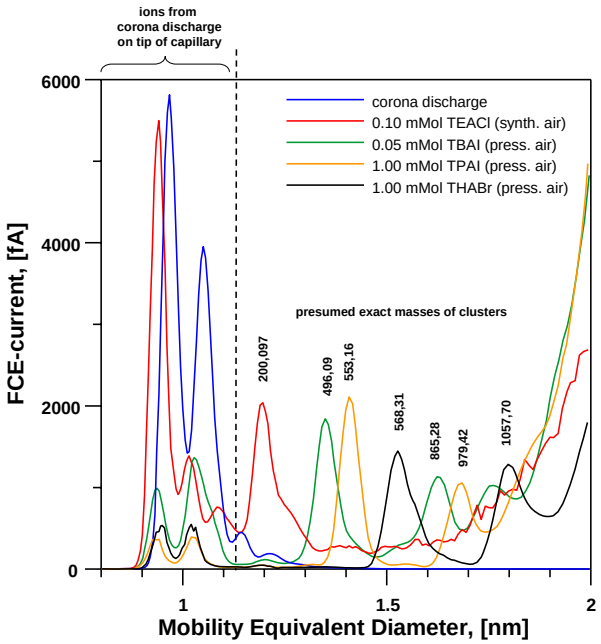

Figure 1: Size spectra of various the tetra-alkyl ammonium halide salts in negative electrospray mode.

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