

Po-210 Charger Ions – Mobility and Mass Investigations and Their Influence on Resulting Bipolar Charge Distributions

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Measurements of nanoparticles in the aerosol phase are often based on electrostatics and thus require charging prior to measurement. For mobility and concentration measurement known charge distributions are a prerequisite. Bipolar charging, using weak radioactive radiation (alpha-, or beta radiation) such as Po-210, Kr-85, Am-241, is the most commonly used charging technique. The radiation ionizes gas molecules via electron loss and attachment of the generated electron to neutral gas molecules. This leads to a close to equal concentration of positively and negatively charged ions. However, as pointed out in previous studies by Steiner et al. (2014), the chemical and physical properties of these ions can change (e.g. depending on gas composition) and thus are likely to be different from setup to setup. The investigation of the nature (mass, mobility) of the charge ions is thus of great interest as it affects the resulting bipolar charge distribution.

Another interesting aspect of charging ions (typically masses of less than 1000 Da, characteristic size less than 2.0nm) is the investigation of the relationship between ion mass linked and ion mobility. An increased interest in new particle formation has led to an increased focus on investigations of sub 2.0 nm particles. An understanding of the relationship between mobility and mass, enabling inference of characteristic size is required to draw clear conclusions from experimental measurements. The existing techniques such as Stokes-Millikan equation, or the regression equations based on measurements by Kilpatrick have recently been found to carry some limitations for small molecular ions (<2.0 nm). Simultaneous mass and mobility measurements coupled with predictions based on precise ion structural models are needed to improve the existing understanding.

In this study we apply differential mobility analysis-mass spectrometry (DMA-MS, with a SEADM P5 DMA and a time of flight mass spectrometer) for simultaneous measurements of positively and negatively charged ions generated by a 10mCi Po-210 source. Some of the measured positively and negatively charged ions were chemically identified using mass identification and the according mobility was derived from DMA measurements. The local energy minimum molecule structures were inferred using density function theory (DFT) calculations (Gaussian Software). These DFT determined structures were applied for mobility prediction calculations using non-specular scattering models. The experimentally found mass to mobility relationship was compared to the calculated relationships and to the Kilpatrick regression equation. Finally, the

bipolar charge distributions from the ion populations generated in our case were calculated applying Brownian dynamics simulations.

The results show that the Kilpatrick regression equation shows good agreement with the experimental mass to mobility results for alcohol chains found as negative charge carrier. However, for polymer based ions such as polytetrafluoroethylene (Teflon) or polydimethylsiloxane the Kilpatrick relationship is underestimating the mobility according to their mass, as is demonstrated in Fig. 1.

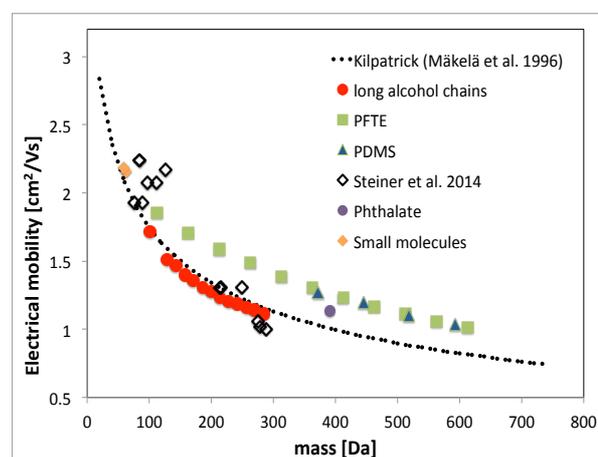


Figure 1. Mobility to Mass relationship, comparison of experimental data, this study and Steiner et al. 2014 and the Kilpatrick regression equation (Mäkelä et al. 1996).

The bipolar charge distribution calculations performed show that the chemical and physical nature of ions barely affects the neutral or singly charged fraction of particles, however, differences are found for different input population in the multiply charged fraction where ion mobility seems to play a non-negligible role.

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