# Experimental studies of the formation of cluster ions formed by corona discharge in an atmosphere containing $SO_2$, $NH_3$, and $H_2O$

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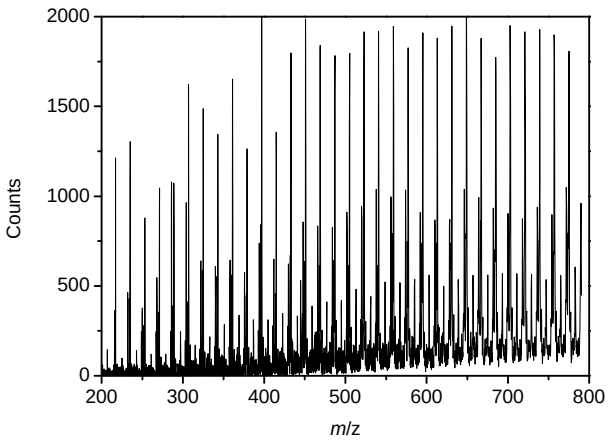
We report on studies of ion induced nucleation in a corona discharge taking place in an atmosphere containing $SO_2$, $NH_3$, and $H_2O$ at standard temperature and pressure. Positive ions such as $H_3O^+(H_2O)_n$, $NH_4^+(H_2O)_n$, and $H^+(H_2SO_4)(H_2O)_n$ and negative ions such as $HSO_5^-(H_2O)_n$, $SO_4^-(H_2O)_n$, $HSO_4^-(H_2O)_n$ and $NO_3^-(H_2O)_n$ have been recorded. Large values of n (> 100) were observed and the experiment indicates the existence of even larger water clusters. In contrast, only clusters with a maximum of 2 sulfuric acid molecules were observed. Fragmentation studies also revealed that the negative ion $HSO_5^-$, which has been observed in many studies, in our experiments is contaminated by $O_2^-(HNO_3)(H_2O)$ ions, and this may also have been the case in other experiments. Finally an ion with *m/z* = 232 (where *m* is the cluster mass in amu and *z* the charge state), capable of attaching $H_2O$-molecules was observed and studied by fragmentation.

The ions were formed by corona discharge in the laboratory atmosphere, where gases such as $SO_2$, $NH_3$, and $H_2O$ could be added to the discharge region. Measurements were done with both positive and negative voltages applied to the discharge needle (relative to the capillary inlet) in order to extract both positive and negative ions. The ions were accelerated by an electrostatic potential of 50 kV. The precursor ions were mass selected with a bending magnet and passed through a gas cell. The product ions exiting the cell were analyzed according to their *m/z*-value, and so called mass-analyzed ion kinetic energy spectra (MIKE) were obtained.

The figure shows an example of the observed distributions. The largest peaks (around 2000 counts) can be identified as $H_3O^+(H_2O)_n$, with n going from 11 to 38. The series with peaks at one mass unit less than the previous series (around 1000 counts) can be identified as $NH_4^+(H_2O)_n$. The series with intensities around 500 counts relates to $H^+(H_2SO_4)(H_2O)_n$.




For the negative ions we also observe the existence of clusters with a very large number of water molecules (n>100). The large clusters are built around a single core ion containing sulfur or $NO_3$.

References:

Hvelplund, P., Pedersen, J.O.P., Støchkel, K., Enghoff, M.B., and Kurtén, T. (2013) *Int. J. Mass. Spectrom. (in press).*