**39th Informal Meeting on Mass Spectrometry**
Paris, France, May 15-17, 2023

# Experimental and theoretical determination of the collision cross sections of phosphoric acid clusters: anions compared to cations

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Electrospray ionization of phosphoric acid solutions readily produces hydrogen bonded phosphoric acid cluster anions and cations, in the negative and positive ion mode, respectively. Using drift tube ion mobility experiments, we determined and compared series of collision cross sections ($^{DT}$CCS) in He and $N_2$ for phosphoric acid cluster anions and cations with different aggregation number n (4 to 90) and different charge states (1 to 4). We obtained different growth rate and CCS properties as a function of the aggregation number (*n*) for positively and negatively charged cluster ions. Then, we set up coarse-grain models using cluster of spheres and theoretical CCS calculations with either the projection approximation or the trajectory methods.

The $^{DT}$CCS values were always found larger for a given aggregation number *n* for positive cluster ions than for negative cluster ions, both in He and in $N_2$ drift gas. The aggregation number *n* for which charge states increased was lower for negative cluster ions than for positive cluster ions, expectedly for cluster of acid molecules.

Using the projection approximation method for CCS calculation in helium, we found that, consistently with the observed trend, the coarse-grain model that fitted negative cluster ions had lower sphere radii than the positive cluster ions.

From this simple aggregation of sphere model, we calculated a charge density for both negative and positive cluster ions and compared it to the Rayleigh limit of the circumscribed sphere.