

Attachment of Water and Alcohol Molecules onto Water and Alcohol Clusters

Isabelle Braud^{* †1}, Julien Boulon^{* †}, Sébastien Zamith^{* †}, and Jean-Marc L'Hermite^{* †}

^{*} Laboratoire Collisions Agrégats Réactivité, IRSAMC, Université de Toulouse, UPS, F-31062 Toulouse, France

[†] CNRS, UMR 5589, F-31062 Toulouse, France

Synopsis We measured the absolute attachment cross-sections of water and alcohol molecules colliding with protonated water and alcohol clusters. Dynamical arguments are used to explain the lower than geometrical cross-sections at small sizes.

By studying the collision between clusters and molecules we can have a better understanding of the growth (nucleation) process. We focused on H-bonded systems such as water, methanol and ethanol that are solvent involved in many physical and chemical processes, in particular as nucleation seeds in atmospheric physics [1].

In the present study we report the measurement of absolute attachment cross-sections of single molecules M (M = water, methanol, or ethanol) onto positively charged mass-selected clusters X_nH^+ (X = water, methanol, or ethanol). Cluster sizes range from tens to hundreds of molecules and the center-of-mass collision energies vary from 0.1 to ~ 1 eV [2].

The attachment cross-sections converge towards the geometrical (hard-sphere) cross-sections at large cluster sizes, whereas they are noticeably lower for small sizes as shown in figure 1.

For homogeneous attachment reactions $X_nH^+ + X \rightarrow X_{n+1}H^+$, this decrease in the cross-section is well explained by a dynamical collisional model. Indeed when the collision time is short compared to the main vibrational period of the cluster's surface vibration mode, the cluster cannot absorb all the collision energy. From our previous results on water [3] and using a mass-scaling, the experimental results are well reproduced for both methanol and ethanol

clusters.

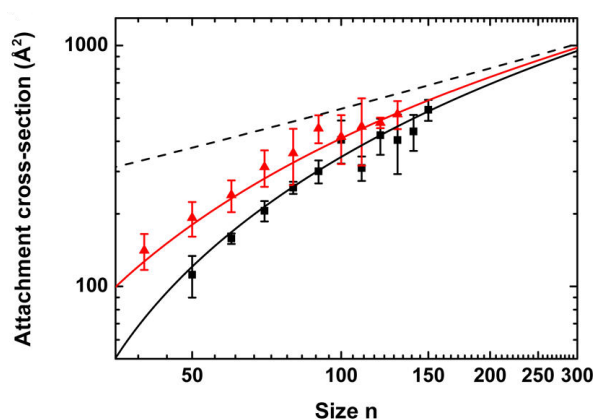


Figure 1. Log-log plot of the attachment cross-sections for methanol molecules onto protonated methanol clusters for two kinetic energies in the laboratory frame [2]. Red triangles: 12 eV. Black squares: 22 eV. Dashed line: geometrical cross-section. Full lines: predictions from the dynamical model.

For inhomogeneous attachment reactions $X_nH^+ + Y \rightarrow X_nYH^+$ (X, Y = water, ethanol, or methanol), however, this simple dynamical model does not satisfactorily account for the measured data, although the global size dependences are qualitatively reproduced.

References

- [1] J. Lengyel *et al* 2012 *J Chem Phys* **137** 034304
- [2] I. Braud *et al* 2015 *J Phys Chem A* doi: 10.1021/jp511854r
- [3] S. Zamith *et al* 2010 *J Chem Phys* **133** 154305

¹E-mail: isabelle.braud@irsamc.ups-tlse.fr

