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Fragmentation of charged aqueous nanodroplets

KENGO ICHIKI, STYLIANI CONSTA, Department of Chemistry, University of Western Ontario — The whole evaporating process of charged aqueous nanodroplets is studied by systematic molecular dynamics simulations until most of the solvent molecules are evaporated. The solvent evaporation makes the droplet smaller and smaller, and at a certain point the repulsive force among ions causes an instability, where typically single ion and 10 to 20 water molecules are disintegrated from the main droplet. This ion fragmentation occurs around 70 to 80% of the charge predicted by the Rayleigh theory [Lord Rayleigh, Phil. Mag. **14**, 184 (1882)]. The numerical results are summarized in the function $R(z)$ which is the fragmentation radius at the charge z. From the fitting by the power law $R \propto z^{\beta}$, we find that at lower temperature $T = 350$ and 370 K the result is close to the Rayleigh theory $\beta = 2/3$, while at higher temperature $T = 400$ and 450 K it is like $\beta = 1/2$. Another fitting on $R(z)$ by the extended ion evaporation mechanism [M. Gamero-Castaño and J. Fernández de la Mora, Anal. Chim. Acta **406**, 67 (2000)] works well for both cases. The final state of the evaporation process is typically a single ion with several water molecules. If we put an alanine dipeptide in zwitterionic form at the beginning, two charges remain in some cases.

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