Stability of multiply-charged clusters: Applications to droplets produced in ESI-MS experiments

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Charged droplets are entities of interest in many research fields from the study of aerosols in atmospheric physics to biomolecules in electrospray ionisation (ESI) experiments. Recently, we developed a set of parallel programs, a classical Monte-Carlo code, called MCMC^2[1], and a molecular dynamics code, called MDMC^2[2], that aim to help determining the structural, thermodynamic, and dynamic properties of multiply-charged clusters, model systems for charged droplets in a coarse-grained representation. The interaction between particles that composed the clusters are based on Lennard-Jones and electrostatic interactions with possible inclusion of polarisation. We will first focus our discussion on the structure and thermodynamics of charged clusters in the size range $55 \leq N \leq 1169$. In particular, we will discuss the influence of temperature, charge values, and number of charged particles on the energy landscape explored during the Monte Carlo simulations and on the distribution of charged particles within the cluster (interior or surface of the cluster)[3]. To shed some light on stability conditions[4] and fragmentation mechanisms of these clusters (Coulomb explosion or fission), heat capacity curves from Monte Carlo simulations will be discussed in conjunction with cluster distortion coefficients and mass spectra derived from dynamics simulations. Some of these structural and dynamic results will be compared to force fields molecular dynamics simulations performed by other groups to model ESI droplets.

References

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