

# How Spherical Are Gaseous Low Charged Dendrimer Ions: a Molecular Dynamics / Ion Mobility Study?

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## Abstract

The globular shape of gaseous ions, resulting from the ionization of large molecules such as polymers and proteins, is a recurring subject that has undergone a renewed interest with the advent of ion mobility spectrometry (IMS), especially in conjunction with theoretical chemistry techniques such as Molecular Dynamics (MD). Globular conformations result from a fine balance between entropy and enthalpy considerations. For multiply charged ions isolated in the gas phase of a mass spectrometer, the Coulombic repulsion between the different charges tends to prevent the ions from adopting a compact, and folded 3D structure. In the present paper, we closely associate data from IMS experiments and MD simulations to unambiguously access the conformations of dendrimer ions in the gas phase with special attention paid to the dendrimer structure, the generation, and the charge state. By doing so, we here combine a set of structural tools able to evaluate the (non)globular shape of ions based on both experimental and theoretical results. The study of dendrimer ions is the first step toward the characterization of the supramolecular complexes formed by electrostatic interactions between polyanionic nucleic acids and polycationic dendrimers called dendriplexes, in the context of gene delivery [1].

## Reference

1. Dufès *et al.*, *Adv. Drug Deliv. Rev.*, **57**, 2177-2202 (2005)